

Ferromagnetism without flat bands in thin armchair nanoribbons

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Abstract

Describing by a Hubbard type of model a thin armchair graphene ribbon in the armchair hexagon chain limit, one shows in exact terms, that even if the system does not have flat bands at all, at low concentration a mesoscopic sample can have ferromagnetic ground state, being metallic in the same time. The mechanism is connected to a common effect of correlations and confinement.

I. INTRODUCTION

Carbon-based nanoscale structures holding hexagonal repeating units and different type of boundaries attract considerable interest by unprecedented application possibilities in the design of organic nanodevices^{1,2}. From these, nanoribbons are of particular interest³, being studied especially because of the emergence possibilities of itinerant ferromagnetism⁴⁻⁶, this subject being also driven by the aim to produce magnetic behavior in organic materials not containing magnetic elements⁷.

In these systems the shape of the edges is either of zig-zag or armchair type⁸. The former case is usually associated to localized edge states⁹ which, due to their high degeneracy, can lead to flat-band ferromagnetism⁴ (in most cases a spin-polarized many particle, but localized ground state). The localized edge states for zig-zag edges on thick samples have been observed experimentally by scanning tunneling microscopy¹⁰, but it is also known that in the thin ribbon case (the chain limit) the localized ferromagnetic nature is no more present in exact terms, and the spin polarized state becomes conducting in the low concentration limit for mesoscopic samples¹¹. Nevertheless, the emergence possibility of the edge localized states for zig-zag boundaries directed the attention to the armchair edges in the search for itinerant ferromagnetism in these structures.

For armchair carbon-based nanoribbons the bulk states and the localized end states are considered entangled by the short-range Coulomb repulsion⁴. In these conditions, at the level of theoretical predictions, itinerant carriers in dispersive bands are supposed to mediate via exchange coupling the interaction among the local magnetic moments present in flat bands^{5,6}. Different approximate techniques are used for the description as: effective field theories combined with variational wave function approach⁵, or analytical weak-coupling analysis combined with numerical density matrix renormalization-group method and first-principles calculations⁶. As a general observation one notes that the deduced results attract the attention to the importance of the Coulomb interaction and correlation effects in providing the physical properties of the systems under study^{4,6,12}. This information is important also in a broader context, since for example, potential nanoribbon applications in building up organic transistors or spin qubits^{13,14} do not take into account correlation effects at all.

On the theoretical side the studies directed to the explanation of ferromagnetism are in a stage present at other organic systems as well, for example pentagon chains⁷, where the initial

attempts based on flat band ferromagnetism¹⁵ encounter the difficulties of this model. One of these is the fact that a perfectly flat band is difficult to obtain. The second difficulty is related to the observation that the connectivity condition needed for the flat band ferromagnetism, is often not satisfied in experimentally manageable situations¹⁶, and this case is encountered for armchair nanoribbons as well⁶. The corrected theory in the light of this new input is usually a some kind of developed flat band theory which does not need the in-flat-band connectivity condition. On this line, for example in the case of the pentagon chains, a model applied in describing rare earth compounds has been suggested to work¹⁶ using strong hybridization effects¹⁷, while in the case of the armchair nanoribbons constructed from hexagon cells, electrons from dispersive bands are conjectured to interconnect the moments created inside the flat bands^{5,6}. In fact, this last possibility is also known in the literature. In $D = 1$ one dimensional case it originates from Ref.¹⁸, whose extended version to $D > 1$ can be find in Ref.¹⁹.

All the previously mentioned results relating ferromagnetism in organic nanoribbons suggest that spin-polarized states in such systems are intimately connected to bare flat bands. This suggestion focuses the research directed to the understanding of ferromagnetism (and this is the case also for graphene structures) exclusively on flat band emergence possibilities, in condition when it is known that systems built up from hexagonal cells containing several sublattices, usually do not contain flat bands^{11,20}, and flat bands are possible to appear only in special conditions, for example as consequences of edge states. Given by the importance of the application possibilities of such organic systems in various fields of nanotechnology, this state of facts naturally leads to a main question: are indeed flat bands necessary for the emergence of ferromagnetism in structures built up from repeating hexagonal units ? Guided by this question, with the aim to provide relevant information and advancement in this field, one shows below in exact terms, that the answer to this question is negative.

In order to do that, one chooses the simplest possible armchair nanoribbon, an armchair hexagon chain (see Fig.1) which besides the fact that represents a real existing structure (i.e. polyphenanthrene), represents as well an armchair nanoribbon in the extreme thin limit. One uses for it a realistic Hubbard type of model which takes into account as well the non-zero next nearest neighbor hopping amplitudes²⁰, and different on-site potentials on different type of sites. Even if the system is not integrable, using a special technique one deduces exact ground states for it. These, in the small concentration limit turn out

to be itinerant and ferromagnetic in conditions in which flat bands are completely missing from the system. One shows that the spin polarization emerging for mesoscopic samples is a consequence of the common effect of correlations and confinement. Since increasing the ribbon width there is not present a physical reason to cancel this behavior, we expect similar effect to occur for thicker ribbons as well.

The method one uses is related to positive semidefinite operator properties. Based on these, one transforms the Hamiltonian of the system (\hat{H}) in positive semidefinite form, the ground state being provided by the most general wave vector which gives the minimum possible eigenvalue (i.e. zero) of the positive semidefinite operators building up \hat{H} . The technique itself works well even in unexpected circumstances from the traditional point of view of exact solutions as: three dimensions²¹, disordered and interacting systems in two dimensions²², stripes, checkerboards and droplets in two dimensions²³, delocalization effect of the Hubbard interaction in two dimensions²⁴, ferroelectric systems²⁵, superconductors^{26,27}, or non-integrable chain structures even under the action of external magnetic fields^{28,29}. Different procedures of the method can be find in Refs.³⁰⁻³², and extreme details regarding its application in the case of the chain structures have been presented in Refs.^{28,29}.

One notes that the first exact results for the armchair hexagon chain in the interacting case are contained in this paper. In order to deduce these, a special technique able to handle the emerging extended operators in the presented case has been developed, used, and described.

The remaining part of the paper is organized as follows. Section II. presents in details the studied system, Sect. III. describes the transformation of the Hamiltonian in positive semidefinite form, Sect. IV. deduces the ground state wave function and presents the physical properties of the obtained ferromagnetic phase, Sect. V. containing the summary and conclusions closes the presentation, and the Appendices A-C contain mathematical details.

II. THE SYSTEM

The studied system is an armchair hexagon chain whose cell constructed at the site \mathbf{j} is presented in Fig.1. One has 8 in-cell positions at the sites $\mathbf{j} + \mathbf{r}_\nu$, $\nu = 1, 2, \dots, 8$, \mathbf{a} represents the Bravais vector of the chain, and for mathematical convenience one has $\mathbf{r}_1 = 0$. One further underlines that the ν index denotes as well eight different sublattices S_ν present in

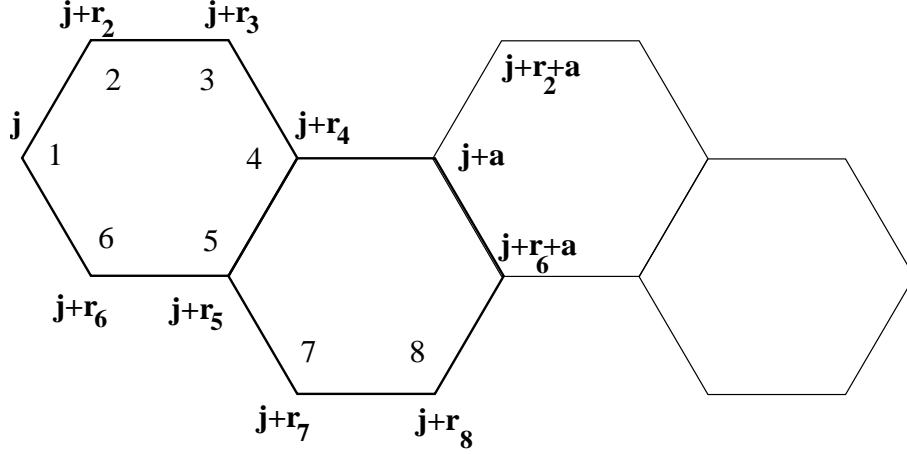


FIG. 1: The armchair hexagonal chain with cell constructed at the site \mathbf{j} (thick line). The in-cell positions are $\mathbf{j}+\mathbf{r}_\nu$, where $\nu = 1, 2, \dots, 8$ is denoting as well eight different sublattices. \mathbf{a} is the Bravais vector, and one has $\mathbf{r}_1 = 0$. The numbers inside the cell represent the ν index of the in-cell sites.

the system.

The Hamiltonian of the system can be written as

$$\hat{H} = \hat{T}_0 + \hat{T}_1 + \hat{T}_2 + \hat{H}_U, \quad (1)$$

where the kinetic part $\hat{H}_0 = \hat{T}_0 + \hat{T}_1 + \hat{T}_2$ contains the contributions of the one-particle local potentials (\hat{T}_0), the nearest neighbor (\hat{T}_1) and the next nearest neighbor (\hat{T}_2) hopping terms, while \hat{H}_U represents the Hubbard interaction. One has

$$\begin{aligned}
\hat{T}_0 &= \sum_{\sigma} \sum_{n=0}^{N_c-1} \{ \epsilon_0 [\hat{n}_{\mathbf{j},\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_4,\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_5,\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_6,\sigma}] \\
&\quad + \epsilon_1 [\hat{n}_{\mathbf{j}+\mathbf{r}_2,\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_3,\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_7,\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_8,\sigma}] \}, \\
\hat{T}_1 &= \sum_{\sigma} \sum_{n=0}^{N_c-1} \{ t_1 [\hat{c}_{\mathbf{j},\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_6,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + H.c.] \\
&\quad + t_2 [\hat{c}_{\mathbf{j}+\mathbf{r}_6,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{a},\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + H.c.] \\
&\quad + t_3 [\hat{c}_{\mathbf{j}+\mathbf{r}_2,\sigma}^{\dagger} \hat{c}_{\mathbf{j},\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_3,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_7,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_6+\mathbf{a},\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_8,\sigma} + H.c.] \\
&\quad + t_4 [\hat{c}_{\mathbf{j}+\mathbf{r}_3,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_2,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_8,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_7,\sigma} + H.c.] \}, \\
\hat{T}_2 &= \sum_{\sigma} \sum_{n=0}^{N_c-1} \{ t'_1 [\hat{c}_{\mathbf{j}+\mathbf{r}_3,\sigma}^{\dagger} \hat{c}_{\mathbf{j},\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_2,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_3,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_2,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_6,\sigma} \\
&\quad + \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_7,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_8,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_7,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_6+\mathbf{a},\sigma} \\
&\quad + \hat{c}_{\mathbf{j}+\mathbf{r}_8,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{a},\sigma} + \hat{c}_{\mathbf{j}+\mathbf{a},\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_3,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_2+\mathbf{a},\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} \\
&\quad + \hat{c}_{\mathbf{j}+\mathbf{r}_7,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_6,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_5+\mathbf{a},\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_8,\sigma} + H.c.] \\
&\quad + t'_2 [\hat{c}_{\mathbf{j},\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_6,\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{a},\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} + \hat{c}_{\mathbf{j}+\mathbf{r}_6+\mathbf{a},\sigma}^{\dagger} \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + H.c.] \}, \\
\hat{H}_U &= \sum_{n=0}^{N_c-1} \{ U_0 [\hat{n}_{\mathbf{j},\sigma} \hat{n}_{\mathbf{j},-\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_4,\sigma} \hat{n}_{\mathbf{j}+\mathbf{r}_4,-\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_5,\sigma} \hat{n}_{\mathbf{j}+\mathbf{r}_5,-\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_6,\sigma} \hat{n}_{\mathbf{j}+\mathbf{r}_6,-\sigma}] \\
&\quad + U_1 [\hat{n}_{\mathbf{j}+\mathbf{r}_2,\sigma} \hat{n}_{\mathbf{j}+\mathbf{r}_2,-\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_3,\sigma} \hat{n}_{\mathbf{j}+\mathbf{r}_3,-\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_7,\sigma} \hat{n}_{\mathbf{j}+\mathbf{r}_7,-\sigma} + \hat{n}_{\mathbf{j}+\mathbf{r}_8,\sigma} \hat{n}_{\mathbf{j}+\mathbf{r}_8,-\sigma}] \}. \quad (2)
\end{aligned}$$

In (2) $\hat{c}_{\mathbf{i},\sigma}^{\dagger}$ creates an electron with spin σ at the site \mathbf{i} , $\hat{n}_{\mathbf{i},\sigma}$ is the particle number operator, N_c represents the number of cells, and during the summation over n , $\mathbf{j} = \mathbf{i} + n\mathbf{a}$ is considered, \mathbf{i} being an arbitrary site of the sublattice $S_{\nu=1}$. The parameters of \hat{H} describing a realistic system are presented in Fig.2. The nearest neighbor hoppings are t_1 (touching bonds between hexagons), t_2 (horizontal hopping on the armchair), t_3 (the oblique hopping on the armchair), and t_4 (the hopping on the external armchair bond). The next nearest neighbor hoppings are t'_1 (bonds with only one end on touching points between hexagons), and t'_2 (bonds with both ends on touching points between hexagons). Furthermore, one notes that the one-particle on-site potentials (ϵ_{α}) and the on site Coulomb repulsions U_{α} are denoted by the index $\alpha = 0$ on the touching points between hexagons, and by the index $\alpha = 1$ on other (external) sites. For mathematical simplicity one considers $U_0 = U_1 = U > 0$, and periodic boundary conditions are taken into account.

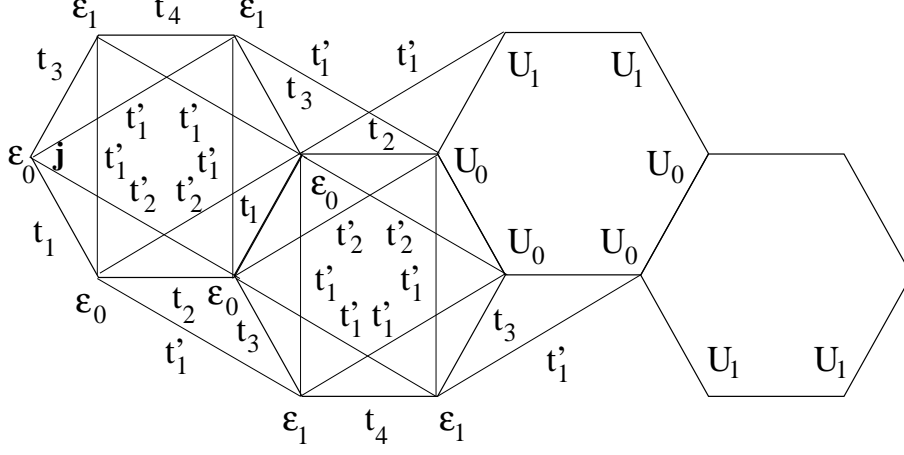


FIG. 2: The Hamiltonian parameters (see text following (2)).

III. THE TRANSFORMATION OF THE HAMILTONIAN IN A POSITIVE SEMIDEFINITE FORM

A. The defined block operators

In order to transform the Hamiltonian (1,2) in a positive semidefinite form one defines eight block operators $\hat{A}_{p,\mathbf{j},\sigma}$, $p = 1, 2, \dots, 8$ for each site \mathbf{j} of the sublattice $\nu = 1$, as follows

$$\begin{aligned}
\hat{A}_{1,\mathbf{j},\sigma} &= a_1 \hat{c}_{\mathbf{j},\sigma} + a_2 \hat{c}_{\mathbf{j}+\mathbf{r}_2,\sigma} + a_3 \hat{c}_{\mathbf{j}+\mathbf{r}_3,\sigma} + a_4 \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} \\
\hat{A}_{2,\mathbf{j},\sigma} &= b_1 \hat{c}_{\mathbf{j},\sigma} + b_4 \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + b_5 \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} + b_6 \hat{c}_{\mathbf{j}+\mathbf{r}_6,\sigma} \\
\hat{A}_{3,\mathbf{j},\sigma} &= d_0 \hat{c}_{\mathbf{j}+\mathbf{a},\sigma} + d_4 \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + d_5 \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} + d_6 \hat{c}_{\mathbf{j}+\mathbf{r}_6+\mathbf{a},\sigma} \\
\hat{A}_{4,\mathbf{j},\sigma} &= e_5 \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} + e_6 \hat{c}_{\mathbf{j}+\mathbf{r}_6+\mathbf{a},\sigma} + e_7 \hat{c}_{\mathbf{j}+\mathbf{r}_7,\sigma} + e_8 \hat{c}_{\mathbf{j}+\mathbf{r}_8,\sigma} \\
\hat{A}_{5,\mathbf{j},\sigma} &= f_0 \hat{c}_{\mathbf{j}+\mathbf{a},\sigma} + f_3 \hat{c}_{\mathbf{j}+\mathbf{r}_3,\sigma} + f_4 \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + f_5 \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} \\
\hat{A}_{6,\mathbf{j},\sigma} &= g_0 \hat{c}_{\mathbf{j}+\mathbf{a},\sigma} + g_2 \hat{c}_{\mathbf{j}+\mathbf{r}_2+\mathbf{a},\sigma} + g_4 \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + g_6 \hat{c}_{\mathbf{j}+\mathbf{r}_6+\mathbf{a},\sigma} \\
\hat{A}_{7,\mathbf{j},\sigma} &= h_0 \hat{c}_{\mathbf{j}+\mathbf{a},\sigma} + h_5 \hat{c}_{\mathbf{j}+\mathbf{r}_5+\mathbf{a},\sigma} + h_6 \hat{c}_{\mathbf{j}+\mathbf{r}_6+\mathbf{a},\sigma} + h_8 \hat{c}_{\mathbf{j}+\mathbf{r}_8,\sigma} \\
\hat{A}_{8,\mathbf{j},\sigma} &= k_4 \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + k_5 \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} + k_6 \hat{c}_{\mathbf{j}+\mathbf{r}_6,\sigma} + k_7 \hat{c}_{\mathbf{j}+\mathbf{r}_7,\sigma}.
\end{aligned} \tag{3}$$

As seen from (3) the used block operators $\hat{A}_{p,\mathbf{j},\sigma}$ are linear combinations of the starting fermionic operators $\hat{c}_{\mathbf{i},\sigma}$ acting on the sites of the block p defined at the site \mathbf{j} (see Figs.3-10). The numerical prefactors $a_i, b_i, d_i, \dots, k_i$ are unknown at the moment, and will be deduced further on.

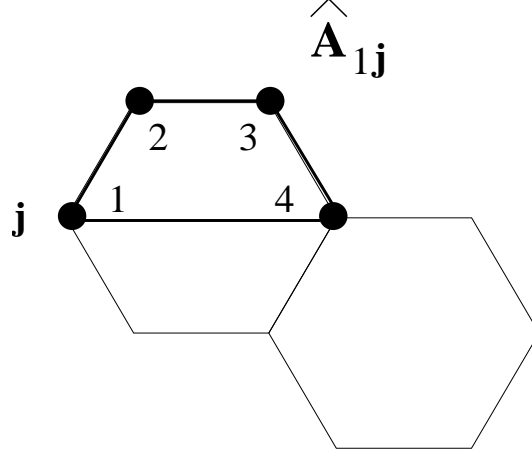


FIG. 3: The block $p = 1$ depicted in the cell defined at the site \mathbf{j} providing the block operator $\hat{A}_{1,\mathbf{j},\sigma}$. The thick line shows the block, while the numbers are indicating the ν index of the sites whose position is $\mathbf{j} + \mathbf{r}_\nu$.

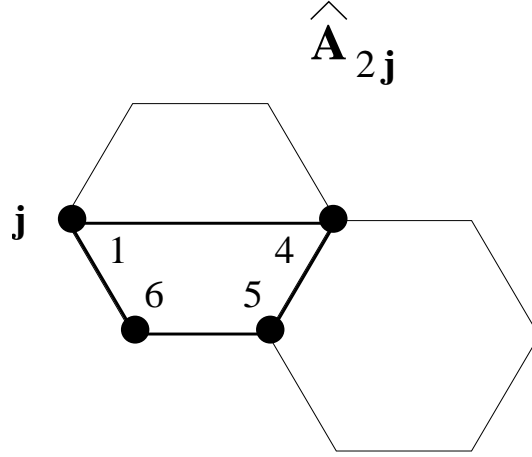


FIG. 4: The block $p = 2$ depicted in the cell defined at the site \mathbf{j} providing the block operator $\hat{A}_{2,\mathbf{j},\sigma}$. The thick line shows the block, while the numbers are indicating the ν index of the sites whose position is $\mathbf{j} + \mathbf{r}_\nu$.

B. The positive semidefinite form of the Hamiltonian

Based on the block operators defined in (3), the starting Hamiltonian presented in (1,2) is transformed (i.e. is rewritten in exact terms) in the following positive semidefinite form

$$\hat{H} = \sum_{\sigma} \sum_{p=1}^8 \sum_{\mathbf{j}=1}^{N_c} \hat{A}_{p,\mathbf{j},\sigma}^{\dagger} \hat{A}_{p,\mathbf{j},\sigma} + \hat{H}_U + K \hat{N}, \quad (4)$$

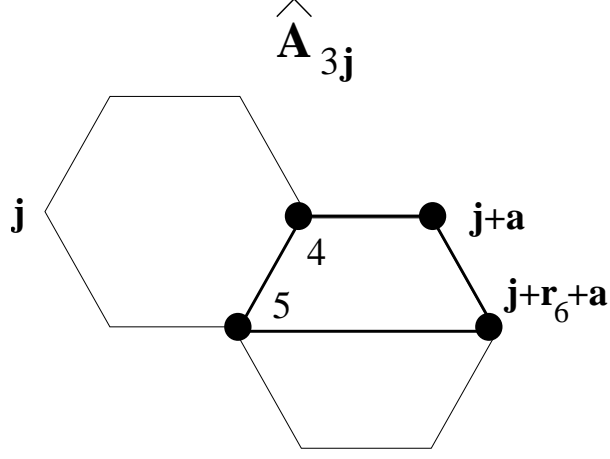


FIG. 5: The block $p = 3$ depicted in the cell defined at the site \mathbf{j} providing the block operator $\hat{A}_{3,\mathbf{j},\sigma}$. The thick line shows the block, while the numbers are indicating the ν index of the sites connected exclusively to a single cell.

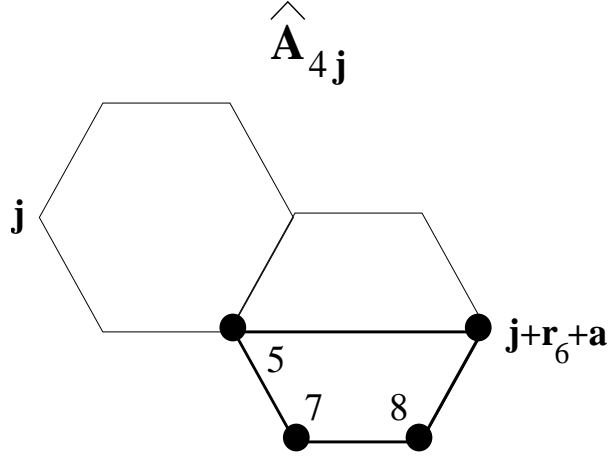


FIG. 6: The block $p = 4$ depicted in the cell defined at the site \mathbf{j} providing the block operator $\hat{A}_{4,\mathbf{j},\sigma}$. The thick line shows the block, while the numbers are indicating the ν index of the sites connected exclusively to a single cell.

where \hat{N} represents the operator of the total number of electrons and K is a constant. The numerical prefactors in (3) and the constant K are expressed by i) effectuating the products $\hat{A}_{p,\mathbf{j},\sigma}^\dagger \hat{A}_{p,\mathbf{j},\sigma}$ and the prescribed sums in the first term of (4), and ii) equating the obtained result term by term to the expression of the starting Hamiltonian (1,2). The obtained equations connecting the parameters of the starting Hamiltonian to the parameters of the block operators and the constant K in the transcribed Hamiltonian (4) are the following

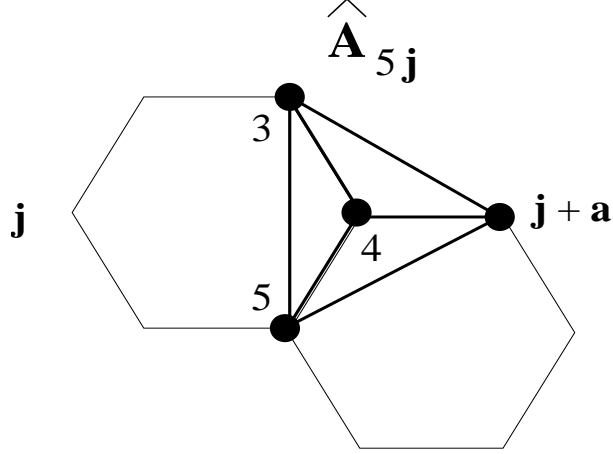


FIG. 7: The block $p = 5$ depicted in the cell defined at the site \mathbf{j} providing the block operator $\hat{A}_{5,\mathbf{j},\sigma}$. The thick line shows the block, while the numbers are indicating the ν index of the sites whose position is $\mathbf{j} + \mathbf{r}_\nu$.

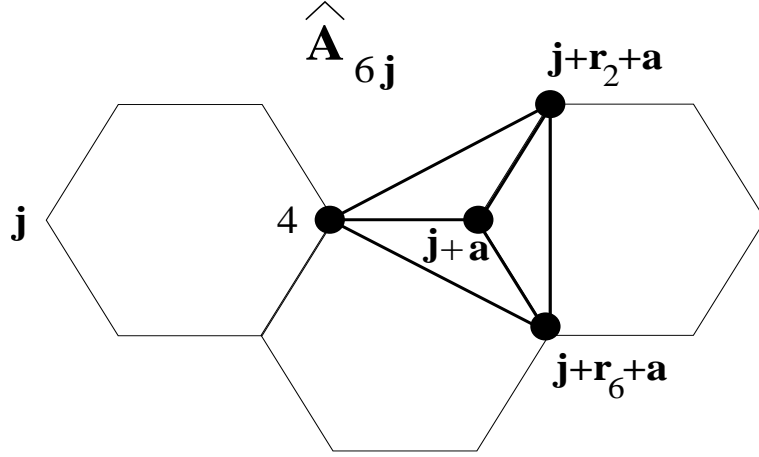


FIG. 8: The block $p = 6$ depicted in the cell defined at the site \mathbf{j} providing the block operator $\hat{A}_{6,\mathbf{j},\sigma}$. The thick line shows the block, the number four indicates the $\nu = 4$ site. Other block sites (placed in the following cell) are indicated by their position $\mathbf{j} + \mathbf{r}_\nu + \mathbf{a}$.

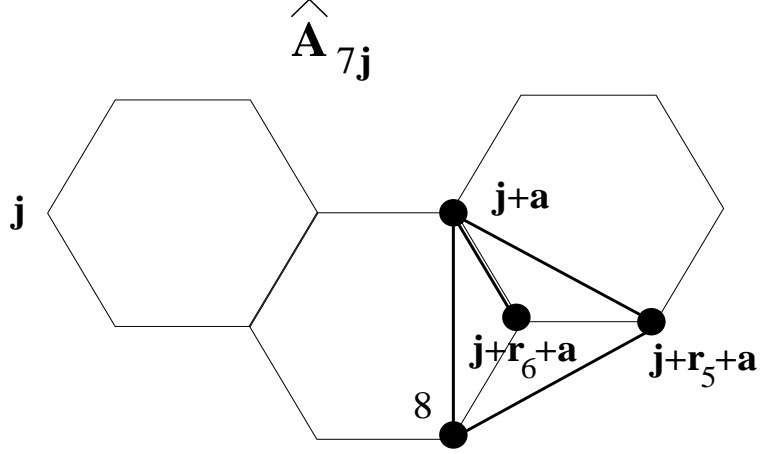


FIG. 9: The block $p = 7$ depicted in the cell defined at the site \mathbf{j} providing the block operator $\hat{A}_{7,\mathbf{j},\sigma}$. The thick line shows the block, the number eight indicates the $\nu = 8$ site. Other block sites (placed in the following cell) are indicated by their position $\mathbf{j} + \mathbf{r}_\nu + \mathbf{a}$.

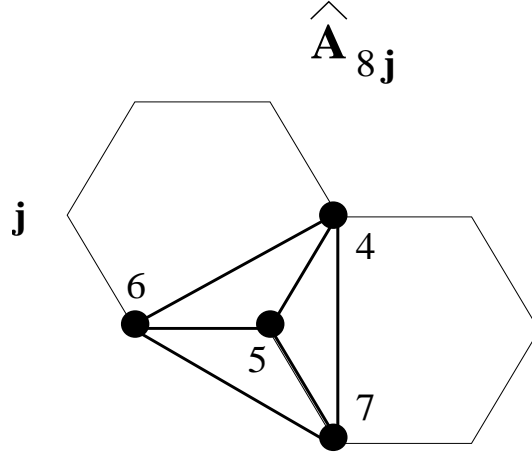


FIG. 10: The block $p = 8$ depicted in the cell defined at the site \mathbf{j} providing the block operator $\hat{A}_{8,\mathbf{j},\sigma}$. The thick line shows the block, while the numbers are indicating the ν index of the sites whose position is $\mathbf{j} + \mathbf{r}_\nu$.

ones: The hopping terms become expressed as

$$\begin{aligned}
t_{\mathbf{j}+\mathbf{r}_5, \mathbf{j}+\mathbf{r}_4} &= t_1 = b_5^* b_4 + d_5^* d_4 + f_5^* f_4 + k_5^* k_4, & t_{\mathbf{j}+\mathbf{r}_1, \mathbf{j}+\mathbf{r}_6} &= t_1 = b_1^* b_6 + g_0^* g_6 + h_0^* h_6 + d_0^* d_6, \\
t_{\mathbf{j}+\mathbf{r}_6, \mathbf{j}+\mathbf{r}_5} &= t_2 = b_6^* b_5 + h_6^* h_5 + k_6^* k_5, & t_{\mathbf{j}+\mathbf{r}_1+\mathbf{a}, \mathbf{j}+\mathbf{r}_4} &= t_2 = d_0^* d_4 + f_0^* f_4 + g_0^* g_4, \\
t_{\mathbf{j}+\mathbf{r}_2, \mathbf{j}+\mathbf{r}_1} &= t_3 = a_2^* a_1 + g_2^* g_0, & t_{\mathbf{j}+\mathbf{r}_4, \mathbf{j}+\mathbf{r}_3} &= t_3 = a_4^* a_3 + f_4^* f_3, \\
t_{\mathbf{j}+\mathbf{r}_6+\mathbf{a}, \mathbf{j}+\mathbf{r}_8} &= t_3 = e_6^* e_8 + h_6^* h_8, & t_{\mathbf{j}+\mathbf{r}_7, \mathbf{j}+\mathbf{r}_5} &= t_3 = e_7^* e_5 + k_7^* k_5, \\
t_{\mathbf{j}+\mathbf{r}_3, \mathbf{j}+\mathbf{r}_2} &= t_4 = a_3^* a_2, & t_{\mathbf{j}+\mathbf{r}_8, \mathbf{j}+\mathbf{r}_7} &= t_4 = e_8^* e_7, & t_{\mathbf{j}+\mathbf{r}_3, \mathbf{j}+\mathbf{r}_1} &= t'_1 = a_3^* a_1, \\
t_{\mathbf{j}+\mathbf{r}_5, \mathbf{j}+\mathbf{r}_3} &= t'_1 = f_5^* f_3, & t_{\mathbf{j}+\mathbf{r}_4, \mathbf{j}+\mathbf{r}_2} &= t'_1 = a_4^* a_2, & t_{\mathbf{j}+\mathbf{r}_2, \mathbf{j}+\mathbf{r}_6} &= t'_1 = g_2^* g_6, \\
t_{\mathbf{j}+\mathbf{r}_8, \mathbf{j}+\mathbf{r}_1+\mathbf{a}} &= t'_1 = h_8^* h_0, & t_{\mathbf{j}+\mathbf{r}_5, \mathbf{j}+\mathbf{r}_8} &= t'_1 = e_5^* e_8, & t_{\mathbf{j}+\mathbf{r}_4, \mathbf{j}+\mathbf{r}_7} &= t'_1 = k_4^* k_7, \\
t_{\mathbf{j}+\mathbf{r}_7, \mathbf{j}+\mathbf{r}_6} &= t'_1 = k_7^* k_6, & t_{\mathbf{j}+\mathbf{r}_7, \mathbf{j}+\mathbf{r}_6+\mathbf{a}} &= t'_1 = e_7^* e_6, & t_{\mathbf{j}+\mathbf{r}_1+\mathbf{a}, \mathbf{j}+\mathbf{r}_3} &= t'_1 = f_0^* f_3, \\
t_{\mathbf{j}+\mathbf{r}_2+\mathbf{a}, \mathbf{j}+\mathbf{r}_4} &= t'_1 = g_2^* g_4, & t_{\mathbf{j}+\mathbf{r}_5+\mathbf{a}, \mathbf{j}+\mathbf{r}_8} &= t'_1 = h_5^* h_8, & t_{\mathbf{j}+\mathbf{r}_6+\mathbf{a}, \mathbf{j}+\mathbf{r}_4} &= t'_2 = d_6^* d_4 + g_6^* g_4, \\
t_{\mathbf{j}+\mathbf{r}_1, \mathbf{j}+\mathbf{r}_5} &= t'_2 = b_1^* b_5 + h_0^* h_5, & t_{\mathbf{j}+\mathbf{r}_6, \mathbf{j}+\mathbf{r}_4} &= t'_2 = b_6^* b_4 + k_6^* k_4, \\
t_{\mathbf{j}+\mathbf{r}_1+\mathbf{a}, \mathbf{j}+\mathbf{r}_5} &= t'_2 = d_0^* d_5 + f_0^* f_5, \\
t_{\mathbf{j}+\mathbf{r}_6+\mathbf{a}, \mathbf{j}+\mathbf{r}_5} &= 0 = d_6^* d_5 + e_6^* e_5, & t_{\mathbf{j}+\mathbf{r}_4, \mathbf{j}+\mathbf{r}_1} &= 0 = a_4^* a_1 + b_4^* b_1,
\end{aligned} \tag{5}$$

while the on-site potentials are given by

$$\begin{aligned}
\epsilon_{\mathbf{j}+\mathbf{r}_1} &= \epsilon_0 = |a_1|^2 + |b_1|^2 + |d_0|^2 + |f_0|^2 + |g_0|^2 + |h_0|^2 + K, \\
\epsilon_{\mathbf{j}+\mathbf{r}_2} &= \epsilon_1 = |a_2|^2 + |g_2|^2 + K, \\
\epsilon_{\mathbf{j}+\mathbf{r}_3} &= \epsilon_1 = |a_3|^2 + |f_3|^2 + K, \\
\epsilon_{\mathbf{j}+\mathbf{r}_4} &= \epsilon_0 = |a_4|^2 + |b_4|^2 + |d_4|^2 + |f_4|^2 + |g_4|^2 + |k_4|^2 + K, \\
\epsilon_{\mathbf{j}+\mathbf{r}_5} &= \epsilon_0 = |b_5|^2 + |d_5|^2 + |e_5|^2 + |f_5|^2 + |h_5|^2 + |k_5|^2 + K, \\
\epsilon_{\mathbf{j}+\mathbf{r}_6} &= \epsilon_0 = |b_6|^2 + |d_6|^2 + |e_6|^2 + |g_6|^2 + |h_6|^2 + |k_6|^2 + K, \\
\epsilon_{\mathbf{j}+\mathbf{r}_7} &= \epsilon_1 = |e_7|^2 + |k_7|^2 + K, \\
\epsilon_{\mathbf{j}+\mathbf{r}_8} &= \epsilon_1 = |e_8|^2 + |h_8|^2 + K.
\end{aligned} \tag{6}$$

For clarity, in (5) one specifies also the hopping matrix elements $t_{\mathbf{i}_1, \mathbf{i}_2}$, as the component of $t_{\mathbf{i}_1, \mathbf{i}_2} \hat{c}_{\mathbf{i}_1, \sigma}^\dagger \hat{c}_{\mathbf{i}_2, \sigma}$ kinetic energy term which leads to the respective equation. Again for clarity, at the level of the on-site potentials in (6), in the index of $\epsilon_{\mathbf{i}}$, the site \mathbf{i} where the analyzed potential is considered is precisely indicated.

One notes that Eqs.(5,6) are the matching conditions of the solution since the transformation from (1,2) to (4) is valid only if Eqs.(5,6) are satisfied.

C. The explicit expression of the operators $\hat{A}_{p,j,\sigma}$

The explicit expression of the transformed Hamiltonian in (4), hence also the explicit form of the $\hat{A}_{p,j,\sigma}$ operators, can be find by solving the matching conditions (5,6). These are representing 36 coupled nonlinear complex algebraic equations containing 33 unknown variables, namely the numerical prefactors $a_i, b_i, d_i, \dots, k_i$ in (3), (in total 32 variables), and the constant K in (4). Based on the solution deduced in the Appendix A, see (A13), the introduced block operators have the expression

$$\begin{aligned}
\hat{A}_{1,j,\sigma} &= \sqrt{t_4} [(\hat{c}_{j+r_2,\sigma} + \hat{c}_{j+r_3,\sigma}) + \frac{t'_1}{t_4} (\hat{c}_{j,\sigma} + \hat{c}_{j+r_4,\sigma})], \\
\hat{A}_{2,j,\sigma} &= \sqrt{t_4} [(\frac{t'_2}{t'_1} - \frac{t_1 + 2t'_2}{2t_3}) (\hat{c}_{j+r_5,\sigma} - \hat{c}_{j+r_6,\sigma}) + \frac{t'_1}{t_4} (\hat{c}_{j,\sigma} - \hat{c}_{j+r_4,\sigma})], \\
\hat{A}_{3,j,\sigma} &= \sqrt{t_4} [(\frac{t'_2}{t'_1} - \frac{t_1 + 2t'_2}{2t_3}) (\hat{c}_{j+a,\sigma} - \hat{c}_{j+r_4,\sigma}) + \frac{t'_1}{t_4} (\hat{c}_{j+r_5,\sigma} - \hat{c}_{j+r_6+a,\sigma})], \\
\hat{A}_{4,j,\sigma} &= \sqrt{t_4} [(\hat{c}_{j+r_7,\sigma} + \hat{c}_{j+r_8,\sigma}) + \frac{t'_1}{t_4} (\hat{c}_{j+r_5,\sigma} + \hat{c}_{j+r_6+a,\sigma})], \\
\hat{A}_{5,j,\sigma} &= t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} [(\hat{c}_{j+a,\sigma} + \hat{c}_{j+r_5,\sigma}) + \frac{2t_3}{t_1 + 2t'_2} \hat{c}_{j+r_3,\sigma} + \frac{(t_3 - t'_1)}{t'_1} \hat{c}_{j+r_4,\sigma}], \\
\hat{A}_{6,j,\sigma} &= t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} [(\hat{c}_{j+r_4,\sigma} + \hat{c}_{j+r_6+a,\sigma}) + \frac{2t_3}{t_1 + 2t'_2} \hat{c}_{j+r_2+a,\sigma} + \frac{(t_3 - t'_1)}{t'_1} \hat{c}_{j+a,\sigma}], \\
\hat{A}_{7,j,\sigma} &= t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} [(\hat{c}_{j+a,\sigma} + \hat{c}_{j+r_5+a,\sigma}) + \frac{2t_3}{t_1 + 2t'_2} \hat{c}_{j+r_8,\sigma} + \frac{(t_3 - t'_1)}{t'_1} \hat{c}_{j+r_6+a,\sigma}], \\
\hat{A}_{8,j,\sigma} &= t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} [(\hat{c}_{j+r_4,\sigma} + \hat{c}_{j+r_6,\sigma}) + \frac{2t_3}{t_1 + 2t'_2} \hat{c}_{j+r_7,\sigma} + \frac{(t_3 - t'_1)}{t'_1} \hat{c}_{j+r_5,\sigma}].
\end{aligned} \tag{7}$$

The parameter space domain where this solution of the matching conditions is valid is not severely restricted, being given by $t_4 > 0$, $t_3 t'_1 / (t_1 + 2t'_2) > 0$, and (A11), see Appendix A. The constant K present in the transformed Hamiltonian from (4) is given in this case by

$$K = \epsilon_1 - t_4 - \frac{2t_3 t'_1}{(t_1 + 2t'_2)}. \tag{8}$$

One notes that the $\hat{A}_{p,j,\sigma}$ operators present in (7) are Fermi operators, since $\hat{A}_{p,j,\sigma}^\dagger \hat{A}_{p,j,\sigma} = \hat{A}_{p,j,\sigma} \hat{A}_{p,j,\sigma}^\dagger = 0$ is satisfied. But these operators are not canonical Fermi operators, since $\{\hat{A}_{p,j,\sigma}, \hat{A}_{p',j',\sigma'}^\dagger\} \neq \delta_{p,p'} \delta_{j,j'} \delta_{\sigma,\sigma'}$ holds.

IV. THE DEDUCTION OF THE GROUND STATE WAVE FUNCTION

A. The deduction method

Based on (7,8) now one knows the explicit expression of the transformed Hamiltonian (4), hence one starts the deduction of the ground state wave function for it, which is written in the form

$$|\Psi_g\rangle = [\prod_{\alpha \in I} \hat{B}_\alpha^\dagger] |0\rangle. \quad (9)$$

In (9), $|0\rangle$ represents the bare vacuum, \hat{B}_α^\dagger are linear combinations of the starting canonical Fermi creation operators $\hat{c}_{i,\sigma}^\dagger$, α represents an index which labels different \hat{B}^\dagger operators, and I represents the domain from which the α indices must be chosen in order to build up the ground state wave function.

The strategy in deducing the \hat{B}_α^\dagger operators is based on the positive semidefinite structure of \hat{H} from (4), namely on the fact that $\hat{H}' = \hat{H} - K\hat{N} = \hat{H}_A + \hat{H}_U$ is a positive semidefinite operator, where $\hat{H}_A = \sum_\sigma \sum_{p=1}^8 \sum_{\mathbf{j}=1}^{N_c} \hat{H}_{A,p,\mathbf{j},\sigma}$ and $\hat{H}_{A,p,\mathbf{j},\sigma} = \hat{A}_{p,\mathbf{j},\sigma}^\dagger \hat{A}_{p,\mathbf{j},\sigma}$. Consequently, $|\Psi_g\rangle$ is the most general wave vector satisfying the requirement

$$(\hat{H}_A + \hat{H}_U)|\Psi_g\rangle = 0, \quad (10)$$

which, because both \hat{H}_A and \hat{H}_U are independently positive semidefinite, is satisfied only if both $\hat{H}_A|\Psi_g\rangle = 0$, and $\hat{H}_U|\Psi_g\rangle = 0$ hold. But since the kernel $\ker(\hat{O})$, of an operator \hat{O} , is a Hilbert subspace spanned by all vectors $|\phi\rangle$ satisfying $\hat{O}|\phi\rangle = 0$, it results that in order to deduce $|\Psi_g\rangle$ we must deduce the most general wave vectors placed inside

$$\ker(\hat{H}') = \ker(\hat{H}_A) \cap \ker(\hat{H}_U). \quad (11)$$

Concentrating first on $\ker(\hat{H}_A)$, one observes that since $\hat{H}_{A,p,\mathbf{j},\sigma}$ are all positive semidefinite operators for all values of all indices, it results that

$$\begin{aligned} \ker(\hat{H}_A) = & \ker(\hat{H}_{A,p=1,\mathbf{j}_1,\uparrow}) \cap \ker(\hat{H}_{A,p=1,\mathbf{j}_1,\downarrow}) \cap \ker(\hat{H}_{A,p=2,\mathbf{j}_1,\uparrow}) \cap \ker(\hat{H}_{A,p=2,\mathbf{j}_1,\downarrow}) \cap \dots \\ & \dots \cap \ker(\hat{H}_{A,p=8,\mathbf{j}_{N_c},\uparrow}) \cap \ker(\hat{H}_{A,p=8,\mathbf{j}_{N_c},\downarrow}), \end{aligned} \quad (12)$$

where, in the right side of the equality, all indices p, \mathbf{j}, σ occur.

Furthermore, one knows that for fixed $p = p', \mathbf{j} = \mathbf{j}', \sigma = \sigma'$ indices, $\ker(\hat{H}_{A,p',\mathbf{j}',\sigma'})$ is spanned by vectors of the form $|\Psi_{A,p',\mathbf{j}',\sigma'}\rangle = \prod_{\alpha \in I_{A,p',\mathbf{j}',\sigma'}} \hat{B}_\alpha^\dagger |0\rangle$ where $I_{A,p',\mathbf{j}',\sigma'}$ collects all α

indices for which the anti-commutation relation $\{\hat{A}_{p',\mathbf{j}',\sigma'}, \hat{B}_\alpha^\dagger\} = 0$ holds²⁹. Indeed in this case $\hat{H}_{A,p',\mathbf{j}',\sigma'}|\Psi_{A,p',\mathbf{j}',\sigma'}\rangle = \hat{A}_{p',\mathbf{j}',\sigma'}^\dagger \hat{A}_{p',\mathbf{j}',\sigma'} \prod_{\alpha \in I_{A,p',\mathbf{j}',\sigma'}} \hat{B}_\alpha^\dagger |0\rangle = 0$ is satisfied, since based on the prescribed anti-commutation relation $\hat{A}_{p',\mathbf{j}',\sigma'} \hat{B}_\alpha^\dagger |0\rangle = -\hat{B}_\alpha^\dagger \hat{A}_{p',\mathbf{j}',\sigma'} |0\rangle = 0$, which given by $\hat{A}_{p',\mathbf{j}',\sigma'} |0\rangle = 0$, is indeed a true relation.

It results that based on (12), the vectors contained in $\ker(\hat{H}_A)$ can be deduced by determining \hat{B}_α^\dagger from the relation

$$\{\hat{A}_{p,\mathbf{j},\sigma}, \hat{B}_\alpha^\dagger\} = 0, \quad (13)$$

where (13) must be satisfied for all values of all indices. One notes that different \hat{B}_α^\dagger solutions of (13) must be linearly independent.

After obtaining the \hat{B}_α^\dagger operators from (13), the domain I present in (9) is such fixed to push $|\Psi_g\rangle$ also in $\ker(\hat{H}_U)$. This last kernel is simply the Hilbert subspace containing all wave vectors with zero double occupancy.

B. The calculation of \hat{B}_α^\dagger operators

1. The \hat{B}_α^\dagger expression

In deducing the \hat{B}_α^\dagger operators one starts from (13) and the already deduced expressions of the $\hat{A}_{p,\mathbf{j},\sigma}$ block operators presented in (7). One considers

$$\hat{B}_\alpha^\dagger = \sum_{\mathbf{i} \in \mathcal{D}_{B_\alpha}} x_{\alpha,\mathbf{i}} \hat{c}_{\mathbf{i},\sigma_{\mathbf{i}}}^\dagger, \quad (14)$$

where two kind of unknown variables must be determined, namely i) the domain \mathcal{D}_{B_α} on which the operator \hat{B}_α^\dagger is defined, and ii) the numerical prefactors $x_{\alpha,\mathbf{i}}$ which specify the linear combination on which \hat{B}_α^\dagger is constructed. After fixing the \hat{B}_α^\dagger expression in (14), the equation (13) must be written for all $\hat{A}_{p,\mathbf{j},\sigma}$ block operators, obtaining a coupled system of $16N_c$ equations which must be solved.

In performing this job one observes the following properties. a) The domain \mathcal{D}_{B_α} cannot be restricted (e.g. extended over $N_b < N_c$ cells). The reason for this is that for restricted \mathcal{D}_{B_α} , we always find at least one $\hat{A}_{p,\mathbf{j},\sigma}$ operator (holding some fixed indices $p = p', \mathbf{j} = \mathbf{j}', \sigma = \sigma'$) which touches the \hat{B}_α^\dagger operator only in a single point \mathbf{j}^* . In this case, since only one kind

of starting fermionic operator is acting on each site and $\{\hat{c}_{\mathbf{j}^*,\sigma}, \hat{c}_{\mathbf{j}^*,\sigma}^\dagger\} = 1$ holds, it results that $\{\hat{A}_{p',\mathbf{j}',\sigma'}, \hat{B}_\alpha^\dagger\} = 0$ cannot be satisfied. Consequently, the \hat{B}_α^\dagger operators will be extended operators (i.e. the domain \mathcal{D}_{B_α} will be extended along the whole system). b) For similar reasons it is not possible to have in the expression of \hat{B}_α^\dagger operators islands of $\hat{c}_{\mathbf{i}',\sigma'}^\dagger$ operators in the background of $\hat{c}_{\mathbf{i},\sigma}^\dagger$ operators where $\sigma' \neq \sigma$. Consequently, for a given \hat{B}_α^\dagger in (14) all $\sigma_{\mathbf{i}}$ indices become fixed, hence $\sigma_{\mathbf{i}} = \sigma$ holds.

Given by these properties, the α index in (14) specifies in fact a fixed spin index σ , and a label index ℓ which numbers the possible \hat{B}^\dagger operators, hence $\alpha = (\ell, \sigma)$, and the expression of the \hat{B}^\dagger operators from (14) becomes

$$\hat{B}_{\ell,\sigma}^\dagger = \sum_{\mathbf{i}} x_{\ell,\mathbf{i}} \hat{c}_{\mathbf{i},\sigma}^\dagger, \quad (15)$$

where the \mathbf{i} sum extends over all sites of the system (in all sublattices).

2. The calculation procedure

For the effective calculation of the $x_{\ell,\mathbf{i}}$ numerical prefactors of the extended operators as $\hat{B}_{\ell,\sigma}^\dagger$ present in (15), special techniques are needed. Such a technique has been developed and presented in Ref.¹¹, based on a recursive connection between coefficients in neighboring cells described by a non-symmetric matrix \tilde{R} , the prefactors being deduced via the unity eigenvalues of \tilde{R}^m , m being an arbitrary positive integer. In order to enlarge and develop the techniques applicable in treating extended operators, one presents and uses here another alternative method. This is based on deducing the $\hat{B}_{\ell,\sigma}^\dagger$ operators for a relatively small chain – named test chain – containing m cells, the test chain being closed in a ring by periodic boundary conditions. Once these operators are deduced, the obtained result is used in the description of a long chain containing $M = p \times m$ cells, the long chain being as well treated by periodic boundary conditions, p being an arbitrary positive integer.

In this method first one deduces the linearly independent $\hat{B}_{\ell,\sigma}^\dagger$ operators for the test chain. This last contains m cells, which are in order numbered by the index $n_c = 1, 2, \dots, m$. The coefficients $x_{\ell,\mathbf{i}}$ become in this way $x_{\ell,n_c,\nu}$ where ν denotes the lattice site $\mathbf{j} + \mathbf{r}_\nu$, $\nu = 1, 2, \dots, 8$ inside the n_c th cell defined at the site \mathbf{j} of the S_1 sublattice (see Fig.1). Consequently, in

this notation, by changing the sum over \mathbf{i} in a sum over n_c and ν , (15) becomes

$$\hat{B}_{\ell,\sigma}^\dagger = \sum_{n_{c\mathbf{j}}=1}^m \sum_{\nu=1}^8 x_{\ell,n_{c\mathbf{j}},\nu} \hat{c}_{\mathbf{j}+\mathbf{a}n_{c\mathbf{j}}+\mathbf{r}_{\nu,\sigma}}^\dagger, \quad (16)$$

where \mathbf{j} is an arbitrary site of the sublattice S_1 . Based on (16) and (3), the anti-commutation relation (13) provides the following system of equations for the prefactors of the $\hat{B}_{\ell,\sigma}^\dagger$ operators

$$\begin{aligned} a_1 x_{\ell,1,1} + a_2 x_{\ell,1,2} + a_3 x_{\ell,1,3} + a_4 x_{\ell,1,4} &= 0, \\ b_1 x_{\ell,1,1} + b_4 x_{\ell,1,4} + b_5 x_{\ell,1,5} + b_6 x_{\ell,1,6} &= 0, \\ d_0 x_{\ell,2,1} + d_4 x_{\ell,1,4} + d_5 x_{\ell,1,5} + d_6 x_{\ell,2,6} &= 0, \\ e_5 x_{\ell,1,5} + e_6 x_{\ell,2,6} + e_7 x_{\ell,1,7} + e_8 x_{\ell,1,8} &= 0, \\ f_0 x_{\ell,2,1} + f_3 x_{\ell,1,3} + f_4 x_{\ell,1,4} + f_5 x_{\ell,1,5} &= 0, \\ g_0 x_{\ell,2,1} + g_2 x_{\ell,2,2} + g_4 x_{\ell,1,4} + g_6 x_{\ell,2,6} &= 0, \\ h_0 x_{\ell,2,1} + h_5 x_{\ell,2,5} + h_6 x_{\ell,2,6} + h_8 x_{\ell,1,8} &= 0, \\ k_4 x_{\ell,1,4} + k_5 x_{\ell,1,5} + k_6 x_{\ell,1,6} + k_7 x_{\ell,1,7} &= 0, \\ a_1 x_{\ell,2,1} + a_2 x_{\ell,2,2} + a_3 x_{\ell,2,3} + a_4 x_{\ell,2,4} &= 0, \\ b_1 x_{\ell,2,1} + b_4 x_{\ell,2,4} + b_5 x_{\ell,2,5} + b_6 x_{\ell,2,6} &= 0, \\ d_0 x_{\ell,3,1} + d_4 x_{\ell,2,4} + d_5 x_{\ell,2,5} + d_6 x_{\ell,3,6} &= 0, \\ e_5 x_{\ell,2,5} + e_6 x_{\ell,3,6} + e_7 x_{\ell,2,7} + e_8 x_{\ell,2,8} &= 0, \\ f_0 x_{\ell,3,1} + f_3 x_{\ell,2,3} + f_4 x_{\ell,2,4} + f_5 x_{\ell,2,5} &= 0, \\ g_0 x_{\ell,3,1} + g_2 x_{\ell,3,2} + g_4 x_{\ell,2,4} + g_6 x_{\ell,3,6} &= 0, \\ h_0 x_{\ell,3,1} + h_5 x_{\ell,3,5} + h_6 x_{\ell,3,6} + h_8 x_{\ell,2,8} &= 0, \\ k_4 x_{\ell,2,4} + k_5 x_{\ell,2,5} + k_6 x_{\ell,2,6} + k_7 x_{\ell,2,7} &= 0, \\ \dots\dots\dots & \end{aligned}$$

$$\begin{aligned}
a_1 x_{\ell,m,1} + a_2 x_{\ell,m,2} + a_3 x_{\ell,m,3} + a_4 x_{\ell,m,4} &= 0, \\
b_1 x_{\ell,m,1} + b_4 x_{\ell,m,4} + b_5 x_{\ell,m,5} + b_6 x_{\ell,m,6} &= 0, \\
d_0 x_{\ell,1,1} + d_4 x_{\ell,m,4} + d_5 x_{\ell,m,5} + d_6 x_{\ell,1,6} &= 0, \\
e_5 x_{\ell,m,5} + e_6 x_{\ell,1,6} + e_7 x_{\ell,m,7} + e_8 x_{\ell,m,8} &= 0, \\
f_0 x_{\ell,1,1} + f_3 x_{\ell,m,3} + f_4 x_{\ell,m,4} + f_5 x_{\ell,m,5} &= 0, \\
g_0 x_{\ell,1,1} + g_2 x_{\ell,1,2} + g_4 x_{\ell,m,4} + g_6 x_{\ell,1,6} &= 0, \\
h_0 x_{\ell,1,1} + h_5 x_{\ell,1,5} + h_6 x_{\ell,1,6} + h_8 x_{\ell,m,8} &= 0, \\
k_4 x_{\ell,m,4} + k_5 x_{\ell,m,5} + k_6 x_{\ell,m,6} + k_7 x_{\ell,m,7} &= 0,
\end{aligned} \tag{17}$$

where the first eight equations from (17) represent (13) written with the operators from (3) defined in the first cell, the second eight equations from (17) represent (13) written with the operators from (3) defined in the second cell, and so on, the last eight equalities from (17) represent (13) written with the operators from (3) defined in the last m th cell. The coefficients a_i, \dots, k_i are presented in (A12) or (7). One finds in this manner a system of $8m$ linear homogeneous equations for $8m$ unknown variables, the $x_{\ell,n_c,\nu}$ prefactors, ℓ being fixed. Solutions are present only if the determinant of the system (17) is zero. This condition specifies different interconnection possibilities between \hat{H}_0 parameters (e.g. different regions of the parameter space specified by the index γ) in a generic form

$$F_\gamma(\{t_\alpha\}, \{\epsilon_\alpha\}) = 0, \tag{18}$$

where solutions are possible to occur. In (18) the sets $\{t_\alpha\}$ and $\{\epsilon_\alpha\}$ are representing the set of hopping matrix elements, and on-site one-particle potentials, respectively. The study of the physical meaning of the condition (18) shows that since flat bands are not present in the bare band structure (see Appendix B, Eq.(B7) together with explications related to this equation), (18) is not connected to the flat band notion, consequently, the ferromagnetism which will be here deduced is not of flat band type. Instead, (18) specifies regions in the parameter space where the density of states around the minimum system energy value is high.

One given deduced \hat{B}^\dagger operator from (17) receives a fixed ℓ index, for example $\ell = 1$. It has hence the form

$$\hat{B}_{1,\sigma}^\dagger = \sum_{n=1}^m \sum_{\nu=1}^8 x_{1,n,\nu} \hat{c}_{\mathbf{j}+n\mathbf{a}+\mathbf{r}_\nu,\sigma}^\dagger, \tag{19}$$

where \mathbf{j} is an arbitrary site of the sublattice S_1 . The obtained $x_{1,n,\nu}$ coefficients in (19) usually have the following properties: i) are different in different cells, e.g. for $n \neq n'$ one has $x_{1,n,\nu} \neq x_{1,n',\nu}$, and ii) rotating the $\hat{B}_{1,\sigma}^\dagger$ operator by π angle around the axis (the line) of the chain, the prefactors attached to each site change their value, e.g.

$$\begin{aligned} x_{1,n,1} &\neq x_{1,n-1,5}, & x_{1,n,2} &\neq x_{1,n-1,7}, & x_{1,n,3} &\neq x_{1,n-1,8}, & x_{1,n,4} &\neq x_{1,n,6}, \\ x_{1,n,5} &\neq x_{1,n,1}, & x_{1,n,6} &\neq x_{1,n-1,4}, & x_{1,n,7} &\neq x_{1,n,2}, & x_{1,n,8} &\neq x_{1,n,3}. \end{aligned} \quad (20)$$

Given by the properties i), ii), new linearly independent $\hat{B}_{\ell,\sigma}^\dagger$ operators are obtained as follows.

i) One translates all coefficients in (19) with one cell, the procedure being possible to be repeated $m - 1$ times. One obtains in this manner

$$\begin{aligned} \hat{B}_{2,\sigma}^\dagger &= \sum_{n=1}^m \sum_{\nu=1}^8 x_{1,n-1,\nu} \hat{c}_{\mathbf{j}+\mathbf{n}\mathbf{a}+\mathbf{r}_\nu,\sigma}^\dagger, \\ \hat{B}_{3,\sigma}^\dagger &= \sum_{n=1}^m \sum_{\nu=1}^8 x_{1,n-2,\nu} \hat{c}_{\mathbf{j}+\mathbf{n}\mathbf{a}+\mathbf{r}_\nu,\sigma}^\dagger, \\ &\dots\dots\dots \\ \hat{B}_{m,\sigma}^\dagger &= \sum_{n=1}^m \sum_{\nu=1}^8 x_{1,n-m+1,\nu} \hat{c}_{\mathbf{j}+\mathbf{n}\mathbf{a}+\mathbf{r}_\nu,\sigma}^\dagger. \end{aligned} \quad (21)$$

ii) After this step one rotates by π degree around the axis of the chain all operators $\hat{B}_{\ell,\sigma}^\dagger$, $\ell = 1, 2, \dots, m$, obtaining m new linearly independent $\hat{B}_{\ell,\sigma}^\dagger$ operators for which $\ell = m+1, m+2, \dots, 2m$ holds. The expression of a $\hat{B}_{\ell',\sigma}^\dagger$ operator obtained by rotating $\hat{B}_{\ell,\sigma}^\dagger$ from (16) becomes

$$\hat{B}_{\ell',\sigma}^\dagger = \sum_{n_{c\mathbf{j}}=1}^m \sum_{\nu=1}^8 x'_{\ell',n_{c\mathbf{j}},\nu} \hat{c}_{\mathbf{j}+\mathbf{a}n_{c\mathbf{j}}+\mathbf{r}_\nu,\sigma}^\dagger, \quad (22)$$

where \mathbf{j} is an arbitrary site of S_1 , and one has (see also (20))

$$\begin{aligned} x'_{\ell',n,1} &= x_{\ell,n-1,5}, & x'_{\ell',n,2} &= x_{\ell,n-1,7}, & x'_{\ell',n,3} &= x_{\ell,n-1,8}, & x'_{\ell',n,4} &= x_{\ell,n,6}, \\ x'_{\ell',n,5} &= x_{\ell,n,1}, & x'_{\ell',n,6} &= x_{\ell,n-1,4}, & x'_{\ell',n,7} &= x_{\ell,n,2}, & x'_{\ell',n,8} &= x_{\ell,n,3}. \end{aligned} \quad (23)$$

The linear independence of the new operators obtained via (21,22) must be always checked, and the presented procedure leads [for one given solution of (17)] to maximum $2m$ linearly independent $\hat{B}_{\ell,\sigma}^\dagger$ operators for a fixed spin index σ . The described procedure than must

be repeated for all independent solutions of (17) connected to the same parameter space domain (18). Explicit examples for the $m = 6$ case (twelve hexagons connected in six cells) are presented in Appendix C.

The deduced $\hat{B}_{\ell,\sigma}^\dagger$ operators on the test chain containing m cells, can be used for the description of a chain containing $M = p \times m$ cells as well, as stated before, p being an arbitrary integer number. For this, a given $\hat{B}_{\ell,\sigma}^\dagger$ operator (maintaining ℓ and σ fixed) is periodically repeated p times to cover completely the chain containing M cells (treated with periodic boundary conditions). In order to increase the number of linearly independent \hat{B}^\dagger operators relating the same chain containing M cells, one must collect all solutions describing the same parameter space region (18) with different m' values such to reobtain the same fixed M via $M = p' \times m'$, where both p' and m' are integers.

C. The ground state wave function

1. The expression of the ground state

Collecting together all linearly independent $\hat{B}_{\ell,\sigma}^\dagger$ operators deduced in the previous subsection and denoting their number by N_B , one has for $|\Psi(N_B)\rangle = \prod_{\sigma} \prod_{\ell=1}^{N_B} \hat{B}_{\ell,\sigma}^\dagger |0\rangle$ the property

$$\hat{H}_A |\Psi(N_B)\rangle = 0. \quad (24)$$

The equality (24) is a direct consequence of (13) [see also the explications presented just above (13)]. Since the kernel $\ker(\hat{H}_A)$ is intimately connected to (13), it results that in the studied conditions, the wave vector $|\Psi(N_B)\rangle$ is unique in satisfying (24).

The ground state is obtained from $|\Psi(N_B)\rangle$ based on (11) by taking from it the contributions which are present also in $\ker(\hat{H}_U)$, i.e. does not contain double occupancy. Since all $\hat{B}_{\ell,\sigma}^\dagger$ operators are extended along a confined space region defined by the studied chain, different $\hat{B}_{\ell,\sigma}^\dagger$ operators holding different ℓ indices intersect each other on several sites of the system. Consequently, the double occupancy can be avoided only if one fixes to the same value all spin indices of all $\hat{B}_{\ell,\sigma}^\dagger$ operators. This property remains also true if one decreases the number of the \hat{B}^\dagger operators present in the wave vector. Hence, the ground state wave

function at $N \leq N_B$ becomes

$$|\Psi_g(N \leq N_B)\rangle = \prod_{\ell=1}^N \hat{B}_{\ell,\sigma}^\dagger |0\rangle, \quad (25)$$

where σ is fixed. The corresponding ground state energy according to (4) is $E_g = KN$, where the K constant is given in (8). The ground state nature arises since because of the missing double occupancy one has $\hat{H}_U|\Psi_g(N \leq N_B)\rangle = 0$, while because of (24), $\hat{H}_A|\Psi_g(N \leq N_B)\rangle = 0$. Hence indeed $(\hat{H}_A + \hat{H}_U)|\Psi_g(N \leq N_B)\rangle = \hat{H}'|\Psi_g(N \leq N_B)\rangle = 0$ is satisfied.

One further note that the described ferromagnetic ground state emerges in the relatively low concentration limit. For example, using the explicit solution presented in Appendix C in the case of a system with $N_c = 36$ cells (containing 72 hexagons), the number of electrons per cell $N/N_c \leq 0.69$ holds, where $\max(N) = N_B$ is satisfied.

2. Physical properties of the ground state

The deduced ground state (25) is a fully polarized ferromagnet. Besides, it is a conducting state since the operators building up the ground state wave vector are extended, and $\delta\mu = \mu_+ - \mu_- = (E_g(N+1) - E_g(N)) - (E_g(N) - E_g(N-1)) = 0$ holds for $N < N_B$. All itinerant electrons being spin-polarized, such systems are potentially applicable in spintronics devices.

The obtained ferromagnetism is not of flat band type, since as shown in Appendix B, flat bands are not present in the system. The spin polarization occurs since extended operators confined in the restricted space region of the chain touch each other, hence must correlate their spin index in order to reduce the double occupancy. A such type of ferromagnetism is created by the common effect of correlations and confinement, and was observed in other hexagon chains as well¹¹. For the appearance of this phase, besides the confined geometry, the following aspects should be present: a) The operators \hat{B}^\dagger building up the ground state wave vector must be extended. Such a property is not *a priori* a chain characteristics, and several chain examples are known where it does not occur^{28,29,33}. Regarding this property one mentions that always when a such type of behavior was observed for chain structures not possessing flat bands, *external hoppings* (i.e. hopping matrix elements connecting different sites from different neighboring cells – see t'_1 in Fig.2) were present. Consequently, when the hopping terms allow the movement along the whole chain (e.g. cage regions where the hopping amplitudes are missing along a chain section perpendicular to the line of the chain

are not present), this seems to be a sufficient condition preserving the extended nature of \hat{B}^\dagger operators. b) The density of states at and around the minimum one-particle energy should be high. This preserves the presence of the fully saturated ferromagnetic state at arbitrary repulsive U in the low concentration limit and finite chain length in the presented case. The mechanism however surely works (probably with lower U bound) in the thermodynamic limit as well, but the effective proof of this statement remains a challenging problem for further investigations.

One further notes that the described ferromagnetic phase emerges for a sequence of different possible interdependences between hopping amplitudes [see the different $A = (t_1 - 4t'_2)/(t_1 + 2t'_2)$ values presented after Eq.(C5)]. Since it is known that carbon-based nanoribbons are sensitive to uniaxial or shear strains³⁴, and/or external pressure³⁵, the needed interdependences between \hat{H}_0 parameters can be achieved for example by strain effects (see also Ref.³⁶).

V. SUMMARY AND CONCLUSIONS

An armchair hexagon chain (i.e. polyphenanthrene) as a representative of a thin armchair ribbon has been described in exact terms by the use of a technique based on positive semidefinite operator properties. The deduced ground state for mesoscopic samples, in the small concentration limit was shown to be ferromagnetic and metallic. This appears in conditions in which flat bands are not present in the bare band structure of the system, the spin polarization being provided by a common effect of correlations and confinement. Since increasing the ribbon width there are not present physical reasons to cancel in exact terms this behavior, at least for a restricted domain of hopping amplitudes we expect similar effect to occur for thicker ribbons as well.

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Appendix A: The deduction of the numerical prefactors of the $\hat{A}_{p,j,\sigma}$ operators

One starts by using from (5) those 14 equations from which every one contains only two unknown variables. From these, namely

$$\begin{aligned} t_4 &= a_3^* a_2, & t_4 &= e_8^* e_7, & t'_1 &= a_3^* a_1, & t'_1 &= f_5^* f_3, \\ t'_1 &= a_4^* a_2, & t'_1 &= g_2^* g_6, & t'_1 &= h_8^* h_0, & t'_1 &= e_5^* e_8, \\ t'_1 &= k_4^* k_7, & t'_1 &= e_7^* e_6, & t'_1 &= f_0^* f_3, & t'_1 &= g_2^* g_4, \\ t'_1 &= k_7^* k_6, & t'_1 &= h_5^* h_8, \end{aligned} \quad (\text{A1})$$

one finds

$$\begin{aligned} a_1 &= \frac{t'_1}{a_3^*}, & a_2 &= \frac{t_4}{a_3^*}, & a_4 &= \frac{t_1'^*}{t_4^*} a_3, & f_0 &= \frac{t_1'^*}{f_3^*}, & f_5 &= \frac{t_1'^*}{f_3^*}, \\ e_5 &= \frac{t_1'^*}{e_8^*}, & e_6 &= \frac{t'_1}{t_4^*} e_8, & e_7 &= \frac{t_4}{e_8^*}, & g_4 &= \frac{t'_1}{g_2^*}, & g_6 &= \frac{t'_1}{g_2^*}, \\ h_0 &= \frac{t'_1}{h_8^*}, & h_5 &= \frac{t_1'^*}{h_8^*}, & k_4 &= \frac{t_1'^*}{k_7^*}, & k_6 &= \frac{t'_1}{k_7^*}. \end{aligned} \quad (\text{A2})$$

Now one uses from (5) the 10 equations containing respectively four unknown variables, namely

$$\begin{aligned} t_3 &= a_2^* a_1 + g_2^* g_0, & t_3 &= a_4^* a_3 + f_4^* f_3, & t_3 &= e_7^* e_5 + k_7^* k_5, \\ t_3 &= e_6^* e_8 + h_6^* h_8, & t'_2 &= b_1^* b_5 + h_0^* h_5, & t'_2 &= b_6^* b_4 + k_6^* k_4, \\ t'_2 &= d_0^* d_5 + f_0^* f_5, & t'_2 &= d_6^* d_4 + g_6^* g_4, & 0 &= a_4^* a_1 + b_4^* b_1, \\ 0 &= d_6^* d_5 + e_6^* e_5, \end{aligned} \quad (\text{A3})$$

in which, (A2) is introduced, and provides

$$\begin{aligned} b_4 &= -\frac{(t_1'^*)^2}{t_4^* b_1^*}, & b_5 &= \frac{1}{b_1^*} [t'_2 - \frac{(t_1'^*)^2}{|h_8|^2}], & b_6 &= b_1 \frac{t_4}{t_1'^2} [\frac{t_1'^2}{|k_7|^2} - t_2'^*], \\ d_0 &= \frac{1}{d_5^*} [t_2'^* - \frac{|t'_1|^2}{|f_3|^2}], & d_4 &= d_5 \frac{t_4}{(t_1'^*)^2} [\frac{|t'_1|^2}{|g_2|^2} - t'_2], & d_6 &= -\frac{t_1'^2}{t_4^* d_5^*}, \\ f_4 &= \frac{1}{f_3^*} [t_3^* - \frac{t_1'^* |a_3|^2}{t_4^*}], & g_0 &= \frac{1}{g_2^*} [t_3 - \frac{t_1' t_4^*}{|a_3|^2}], & h_6 &= \frac{1}{h_8^*} [t_3^* - \frac{t_1' |e_8|^2}{t_4^*}], \\ k_5 &= \frac{1}{k_7^*} [t_3 - \frac{t_1'^* t_4^*}{|e_8|^2}]. \end{aligned} \quad (\text{A4})$$

After this step one remains with 9 unknown variables ($a_3, b_1, d_5, e_8, f_3, g_2, h_8, k_7$, and K), and 12 equations of the following form

$$\begin{aligned}
t_1 &= b_5^* b_4 + d_5^* d_4 + f_5^* f_4 + k_5^* k_4, & t_1 &= b_1^* b_6 + g_0^* g_6 + h_0^* h_6 + d_0^* d_6, \\
t_2 &= b_6^* b_5 + h_6^* h_5 + k_6^* k_5, & t_2 &= d_0^* d_4 + f_0^* f_4 + g_0^* g_4, \\
\epsilon_0 &= |a_1|^2 + |b_1|^2 + |d_0|^2 + |f_0|^2 + |g_0|^2 + |h_0|^2 + K, \\
\epsilon_0 &= |a_4|^2 + |b_4|^2 + |d_4|^2 + |f_4|^2 + |g_4|^2 + |k_4|^2 + K, \\
\epsilon_0 &= |b_5|^2 + |d_5|^2 + |e_5|^2 + |f_5|^2 + |h_5|^2 + |k_5|^2 + K, \\
\epsilon_0 &= |b_6|^2 + |d_6|^2 + |e_6|^2 + |g_6|^2 + |h_6|^2 + |k_6|^2 + K, \\
\epsilon_1 &= |a_2|^2 + |g_2|^2 + K, & \epsilon_1 &= |a_3|^2 + |f_3|^2 + K, \\
\epsilon_1 &= |e_7|^2 + |k_7|^2 + K, & \epsilon_1 &= |e_8|^2 + |h_8|^2 + K.
\end{aligned} \tag{A5}$$

Using (A2,A4) in (A5), introducing the notations

$$\begin{aligned}
|a_3|^2 &= x, & |d_5|^2 &= z, & |f_3|^2 &= w, & |g_2|^2 &= t, \\
|e_8|^2 &= v, & |b_1|^2 &= y, & |h_8|^2 &= u, & |k_7|^2 &= s,
\end{aligned} \tag{A6}$$

and considering real hopping matrix elements, the remaining system of 12 equations becomes of the form

$$\begin{aligned}
\epsilon_1 &= \frac{t_4^2}{x} + t + K, & \epsilon_1 &= \frac{t_4^2}{v} + s + K, \\
\epsilon_1 &= x + w + K, & \epsilon_1 &= v + u + K, \\
\epsilon_0 &= \frac{t_1'^2}{t} + \frac{t_1'^2}{s} + \frac{t_1'^2 x}{t_4^2} + \frac{t_1'^4}{t_4^2 y} + \frac{1}{w} (t_3 - \frac{t_1' x}{t_4})^2 + \frac{t_4^2 z}{t_1'^4} (\frac{t_1'^2}{t} - t_2')^2 + K, \\
\epsilon_0 &= \frac{t_1'^2}{s} + \frac{t_1'^2}{t} + \frac{t_1'^2 v}{t_4^2} + \frac{t_1'^4}{t_4^2 z} + \frac{1}{u} (t_3 - \frac{t_1' v}{t_4})^2 + \frac{t_4^2 y}{t_1'^4} (\frac{t_1'^2}{s} - t_2')^2 + K, \\
\epsilon_0 &= z + \frac{t_1'^2}{v} + \frac{t_1'^2}{w} + \frac{t_1'^2}{u} + \frac{1}{y} (t_2' - \frac{t_1'}{u})^2 + \frac{1}{s} (t_3 - \frac{t_1' t_4}{v})^2 + K, \\
\epsilon_0 &= y + \frac{t_1'^2}{x} + \frac{t_1'^2}{u} + \frac{t_1'^2}{w} + \frac{1}{z} (t_2' - \frac{t_1'}{w})^2 + \frac{1}{t} (t_3 - \frac{t_1' t_4}{x})^2 + K, \\
t_2 &= \frac{t_4}{t_1'^2} (t_2' - \frac{t_1'}{w}) (\frac{t_1'^2}{t} - t_2') + \frac{t_1'}{w} (t_3 - \frac{t_1' x}{t_4}) + \frac{t_1'}{t} (t_3 - \frac{t_1' t_4}{x}), \\
t_2 &= \frac{t_4}{t_1'^2} (t_2' - \frac{t_1'}{u}) (\frac{t_1'^2}{s} - t_2') + \frac{t_1'}{u} (t_3 - \frac{t_1' v}{t_4}) + \frac{t_1'}{s} (t_3 - \frac{t_1' t_4}{v}), \\
t_1 &= \frac{t_1'^2}{t_4 y} (\frac{t_1'^2}{u} - t_2') + \frac{t_4 z}{t_1'^2} (\frac{t_1'^2}{t} - t_2') + \frac{t_1'}{w} (t_3 - \frac{t_1' x}{t_4}) + \frac{t_1'}{s} (t_3 - \frac{t_1' t_4}{v}), \\
t_1 &= \frac{t_1'^2}{t_4 z} (\frac{t_1'^2}{w} - t_2') + \frac{t_4 y}{t_1'^2} (\frac{t_1'^2}{s} - t_2') + \frac{t_1'}{u} (t_3 - \frac{t_1' v}{t_4}) + \frac{t_1'}{t} (t_3 - \frac{t_1' t_4}{x}). \tag{A7}
\end{aligned}$$

The study of (A7) shows that it provides the same equation for pair of variables. For example if η denotes x or v , one finds the equation

$$\begin{aligned}
t_2 &= \frac{t_4}{t_1'^2} (t_2' - \frac{t_1'}{\epsilon_1 - K - \eta}) (\frac{t_1'^2}{\epsilon_1 - K - \frac{t_4^2}{\eta}} - t_2') \\
&+ \frac{t_1'}{\epsilon_1 - K - \eta} (t_3 - \frac{t_1' \eta}{t_4}) + \frac{t_1'}{\epsilon_1 - K - \frac{t_4^2}{\eta}} (t_3 - \frac{t_1' t_4}{\eta}). \tag{A8}
\end{aligned}$$

Similar equations are possible to deduce for the (y, z) , (u, w) , and (t, s) pairs as well, hence one restricts ourselves below to the class of solutions

$$x = v, \quad y = z, \quad u = w, \quad t = s. \tag{A9}$$

By using (A9) in (A7), (A7) reduces to six equations of the form

$$\begin{aligned}
\epsilon_1 &= \frac{t_4^2}{x} + t + K, \\
\epsilon_1 &= x + w + K, \\
\epsilon_0 &= \frac{2t_1'^2}{t} + \frac{t_1'^2 x}{t_4^2} + \frac{t_1'^4}{t_4^2 z} + \frac{t_1'^2}{w} \left(\frac{t_3}{t_1'} - \frac{x}{t_4} \right)^2 + \frac{t_4^2 z}{t_1'^4} \left(\frac{t_1'^2}{t} - t_2' \right)^2 + K, \\
\epsilon_0 &= z + \frac{t_1'^2}{x} + \frac{2t_1'^2}{w} + \frac{1}{z} \left(t_2' - \frac{t_1'^2}{w} \right)^2 + \frac{t_1'^2}{t} \left(\frac{t_3}{t_1'} - \frac{t_4}{x} \right)^2 + K, \\
t_2 &= -\frac{t_4}{t_1'^2} \left(t_2' - \frac{t_1'^2}{w} \right) \left(t_2' - \frac{t_1'^2}{t} \right) + \frac{t_1'^2}{w} \left(\frac{t_3}{t_1'} - \frac{x}{t_4} \right) + \frac{t_1'^2}{t} \left(\frac{t_3}{t_1'} - \frac{t_4}{x} \right), \\
t_1 &= -\frac{t_1'^2}{t_4 z} \left(t_2' - \frac{t_1'^2}{w} \right) - \frac{t_4 z}{t_1'^2} \left(t_2' - \frac{t_1'^2}{t} \right) + \frac{t_1'^2}{w} \left(\frac{t_3}{t_1'} - \frac{x}{t_4} \right) + \frac{t_1'^2}{t} \left(\frac{t_3}{t_1'} - \frac{t_4}{x} \right). \tag{A10}
\end{aligned}$$

One of the possible solutions of (A10) emerges at $x = v = t_4 > 0$, $z = y = t_1'^2/t_4 > 0$, $t = u = s = w = 2t_3 t_1'/(t_1 + 2t_2') > 0$, $K = \epsilon_1 - t_4 - 2t_3 t_1'/(t_1 + 2t_2')$, and requires

$$\begin{aligned}
t_2 &= \frac{t_1 + 2t_2'}{t_3} (t_3 - t_1') - \frac{t_4}{t_1'^2} \left(t_2' - t_1' \frac{t_1 + 2t_2'}{2t_3} \right)^2, \\
\epsilon_0 - \epsilon_1 &= t_1' \left[\frac{2t_1'}{t_4} - \frac{2t_3}{t_1 + 2t_2'} \right] + t_4 \left[\left(\frac{t_1 + 2t_2'}{2t_3} \right)^2 + \frac{t_2'^2}{t_1'^2} - 1 \right] \\
&\quad + t_1' \frac{t_1 + 2t_2'}{2t_3} \left[\left(\frac{t_3}{t_1'} - 1 \right)^2 - \frac{2t_4 t_2'}{t_1'^2} + 2 \right]. \tag{A11}
\end{aligned}$$

It has the form

$$\begin{aligned}
a_1 &= \frac{t_1'}{\sqrt{t_4}}, \quad a_2 = \sqrt{t_4}, \quad a_3 = \sqrt{t_4}, \quad a_4 = \frac{t_1'}{\sqrt{t_4}}, \\
b_1 &= \frac{t_1'}{\sqrt{t_4}}, \quad b_4 = -\frac{t_1'}{\sqrt{t_4}}, \quad b_5 = \sqrt{t_4} \left(\frac{t_2'}{t_1'} - \frac{t_1 + 2t_2'}{2t_3} \right), \quad b_6 = -\sqrt{t_4} \left(\frac{t_2'}{t_1'} - \frac{t_1 + 2t_2'}{2t_3} \right), \\
d_0 &= \sqrt{t_4} \left(\frac{t_2'}{t_1'} - \frac{t_1 + 2t_2'}{2t_3} \right), \quad d_4 = -\sqrt{t_4} \left(\frac{t_2'}{t_1'} - \frac{t_1 + 2t_2'}{2t_3} \right), \quad d_5 = \frac{t_1'}{\sqrt{t_4}}, \quad d_6 = -\frac{t_1'}{\sqrt{t_4}}, \\
e_5 &= \frac{t_1'}{\sqrt{t_4}}, \quad e_6 = \frac{t_1'}{\sqrt{t_4}}, \quad e_7 = \sqrt{t_4}, \quad e_8 = \sqrt{t_4}, \tag{A12} \\
f_0 &= t_1' \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \quad f_3 = \sqrt{\frac{2t_1' t_3}{t_1 + 2t_2'}}, \quad f_4 = (t_3 - t_1') \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \quad f_5 = t_1' \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \\
g_0 &= (t_3 - t_1') \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \quad g_2 = \sqrt{\frac{2t_1' t_3}{t_1 + 2t_2'}}, \quad g_4 = t_1' \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \quad g_6 = t_1' \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \\
h_0 &= t_1' \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \quad h_5 = t_1' \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \quad h_6 = (t_3 - t_1') \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \quad h_8 = \sqrt{\frac{2t_1' t_3}{t_1 + 2t_2'}}, \\
k_4 &= t_1' \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \quad k_5 = (t_3 - t_1') \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \quad k_6 = t_1' \sqrt{\frac{t_1 + 2t_2'}{2t_1' t_3}}, \quad k_7 = \sqrt{\frac{2t_1' t_3}{t_1 + 2t_2'}}.
\end{aligned}$$

The parameter space region \mathcal{D} where this solution emerges is fixed by Eq.(A11) and the conditions $t_4 > 0$, $t_3 t'_1 / (t_1 + 2t'_2) > 0$. The corresponding $\hat{A}_{p,\mathbf{j},\sigma}$ operators are provided by the following relations

$$\begin{aligned}
\hat{A}_{1,\mathbf{j},\sigma} &= \frac{t'_1}{\sqrt{t_4}} \hat{c}_{\mathbf{j},\sigma} + \sqrt{t_4} \hat{c}_{\mathbf{j}+\mathbf{r}_2,\sigma} + \sqrt{t_4} \hat{c}_{\mathbf{j}+\mathbf{r}_3,\sigma} + \frac{t'_1}{\sqrt{t_4}} \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma}, \\
\hat{A}_{2,\mathbf{j},\sigma} &= \frac{t'_1}{\sqrt{t_4}} \hat{c}_{\mathbf{j},\sigma} - \frac{t'_1}{\sqrt{t_4}} \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + \sqrt{t_4} \left(\frac{t'_2}{t'_1} - \frac{t_1 + 2t'_2}{2t_3} \right) \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} - \sqrt{t_4} \left(\frac{t'_2}{t'_1} - \frac{t_1 + 2t'_2}{2t_3} \right) \hat{c}_{\mathbf{j}+\mathbf{r}_6,\sigma}, \\
\hat{A}_{3,\mathbf{j},\sigma} &= \sqrt{t_4} \left(\frac{t'_2}{t'_1} - \frac{t_1 + 2t'_2}{2t_3} \right) \hat{c}_{\mathbf{j}+\mathbf{a},\sigma} - \sqrt{t_4} \left(\frac{t'_2}{t'_1} - \frac{t_1 + 2t'_2}{2t_3} \right) \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + \frac{t'_1}{\sqrt{t_4}} \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} - \frac{t'_1}{\sqrt{t_4}} \hat{c}_{\mathbf{j}+\mathbf{r}_6+\mathbf{a},\sigma}, \\
\hat{A}_{4,\mathbf{j},\sigma} &= \frac{t'_1}{\sqrt{t_4}} \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} + \frac{t'_1}{\sqrt{t_4}} \hat{c}_{\mathbf{j}+\mathbf{r}_6+\mathbf{a},\sigma} + \sqrt{t_4} \hat{c}_{\mathbf{j}+\mathbf{r}_7,\sigma} + \sqrt{t_4} \hat{c}_{\mathbf{j}+\mathbf{r}_8,\sigma}, \\
\hat{A}_{5,\mathbf{j},\sigma} &= t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{a},\sigma} + \sqrt{\frac{2t'_1 t_3}{t_1 + 2t'_2}} \hat{c}_{\mathbf{j}+\mathbf{r}_3,\sigma} + (t_3 - t'_1) \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma}, \\
\hat{A}_{6,\mathbf{j},\sigma} &= (t_3 - t'_1) \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{a},\sigma} + \sqrt{\frac{2t'_1 t_3}{t_1 + 2t'_2}} \hat{c}_{\mathbf{j}+\mathbf{r}_2+\mathbf{a},\sigma} + t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{r}_6+\mathbf{a},\sigma}, \\
\hat{A}_{7,\mathbf{j},\sigma} &= t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{a},\sigma} + t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{r}_5+\mathbf{a},\sigma} + (t_3 - t'_1) \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{r}_6+\mathbf{a},\sigma} + \sqrt{\frac{2t'_1 t_3}{t_1 + 2t'_2}} \hat{c}_{\mathbf{j}+\mathbf{r}_8,\sigma}, \\
\hat{A}_{8,\mathbf{j},\sigma} &= t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{r}_4,\sigma} + (t_3 - t'_1) \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{r}_5,\sigma} + t'_1 \sqrt{\frac{t_1 + 2t'_2}{2t'_1 t_3}} \hat{c}_{\mathbf{j}+\mathbf{r}_6,\sigma} + \sqrt{\frac{2t'_1 t_3}{t_1 + 2t'_2}} \hat{c}_{\mathbf{j}+\mathbf{r}_7,\sigma}.
\end{aligned} \tag{A13}$$

Appendix B: The bare band structure

In order to obtain the bare band structure of the system, one Fourier transforms $\hat{H}_0 = \hat{T}_0 + \hat{T}_1 + \hat{T}_2$ to \mathbf{k} space by using $\hat{c}_{\mathbf{j}+\mathbf{r}_\nu,\sigma} = (1/\sqrt{N_c}) \sum_{\mathbf{k}} \exp[-i\mathbf{k}(\mathbf{j} + \mathbf{r}_\nu)] \hat{c}_{\nu,\mathbf{k},\sigma}$ (where the sum over \mathbf{k} represents a sum over N_c cells), obtaining

$$\begin{aligned}
\hat{T}_0 &= \sum_{\sigma} \sum_{\mathbf{k}} [\epsilon_0 (\hat{c}_{1,\mathbf{k},\sigma}^{\dagger} \hat{c}_{1,\mathbf{k},\sigma} + \hat{c}_{4,\mathbf{k},\sigma}^{\dagger} \hat{c}_{4,\mathbf{k},\sigma} + \hat{c}_{5,\mathbf{k},\sigma}^{\dagger} \hat{c}_{5,\mathbf{k},\sigma} + \hat{c}_{6,\mathbf{k},\sigma}^{\dagger} \hat{c}_{6,\mathbf{k},\sigma}) \\
&\quad + \epsilon_1 (\hat{c}_{2,\mathbf{k},\sigma}^{\dagger} \hat{c}_{2,\mathbf{k},\sigma} + \hat{c}_{3,\mathbf{k},\sigma}^{\dagger} \hat{c}_{3,\mathbf{k},\sigma} + \hat{c}_{7,\mathbf{k},\sigma}^{\dagger} \hat{c}_{7,\mathbf{k},\sigma} + \hat{c}_{8,\mathbf{k},\sigma}^{\dagger} \hat{c}_{8,\mathbf{k},\sigma})], \\
\hat{T}_1 &= \sum_{\sigma} \sum_{\mathbf{k}} [t_1 (\hat{c}_{1,\mathbf{k},\sigma}^{\dagger} \hat{c}_{6,\mathbf{k},\sigma} e^{-i\mathbf{k}\mathbf{r}_6} + \hat{c}_{5,\mathbf{k},\sigma}^{\dagger} \hat{c}_{4,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_5-\mathbf{r}_4)}) \\
&\quad + t_2 (\hat{c}_{6,\mathbf{k},\sigma}^{\dagger} \hat{c}_{5,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_6-\mathbf{r}_5)} + \hat{c}_{1,\mathbf{k},\sigma}^{\dagger} \hat{c}_{4,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{a}-\mathbf{r}_4)}) \\
&\quad + t_3 (\hat{c}_{2,\mathbf{k},\sigma}^{\dagger} \hat{c}_{1,\mathbf{k},\sigma} e^{+i\mathbf{k}\mathbf{r}_2} + \hat{c}_{4,\mathbf{k},\sigma}^{\dagger} \hat{c}_{3,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_4-\mathbf{r}_3)} + \hat{c}_{7,\mathbf{k},\sigma}^{\dagger} \hat{c}_{5,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_7-\mathbf{r}_5)} + \hat{c}_{6,\mathbf{k},\sigma}^{\dagger} \hat{c}_{8,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_6+\mathbf{a}-\mathbf{r}_8)}) \\
&\quad + t_4 (\hat{c}_{3,\mathbf{k},\sigma}^{\dagger} \hat{c}_{2,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_3-\mathbf{r}_2)} + \hat{c}_{8,\mathbf{k},\sigma}^{\dagger} \hat{c}_{7,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_8-\mathbf{r}_7)}) + H.c.], \\
\hat{T}_2 &= \sum_{\sigma} \sum_{\mathbf{k}} [t'_1 (\hat{c}_{3,\mathbf{k},\sigma}^{\dagger} \hat{c}_{1,\mathbf{k},\sigma} e^{+i\mathbf{k}\mathbf{r}_3} + \hat{c}_{4,\mathbf{k},\sigma}^{\dagger} \hat{c}_{2,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_4-\mathbf{r}_2)} + \hat{c}_{5,\mathbf{k},\sigma}^{\dagger} \hat{c}_{3,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_5-\mathbf{r}_3)}) \\
&\quad + \hat{c}_{2,\mathbf{k},\sigma}^{\dagger} \hat{c}_{6,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_2-\mathbf{r}_6)} + \hat{c}_{4,\mathbf{k},\sigma}^{\dagger} \hat{c}_{7,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_4-\mathbf{r}_7)} + \hat{c}_{5,\mathbf{k},\sigma}^{\dagger} \hat{c}_{8,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_5-\mathbf{r}_8)}) \\
&\quad + \hat{c}_{7,\mathbf{k},\sigma}^{\dagger} \hat{c}_{6,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_7-\mathbf{r}_6-\mathbf{a})} + \hat{c}_{8,\mathbf{k},\sigma}^{\dagger} \hat{c}_{1,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_8-\mathbf{a})} + \hat{c}_{1,\mathbf{k},\sigma}^{\dagger} \hat{c}_{3,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{a}-\mathbf{r}_3)}) \\
&\quad + \hat{c}_{2,\mathbf{k},\sigma}^{\dagger} \hat{c}_{4,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_2+\mathbf{a}-\mathbf{r}_4)} + \hat{c}_{7,\mathbf{k},\sigma}^{\dagger} \hat{c}_{6,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_7-\mathbf{r}_6)} + \hat{c}_{5,\mathbf{k},\sigma}^{\dagger} \hat{c}_{8,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_5+\mathbf{a}-\mathbf{r}_8)}) \\
&\quad + t'_2 (\hat{c}_{1,\mathbf{k},\sigma}^{\dagger} \hat{c}_{5,\mathbf{k},\sigma} e^{-i\mathbf{k}\mathbf{r}_5} + \hat{c}_{6,\mathbf{k},\sigma}^{\dagger} \hat{c}_{4,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_6-\mathbf{r}_4)} + \hat{c}_{1,\mathbf{k},\sigma}^{\dagger} \hat{c}_{5,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{a}-\mathbf{r}_5)}) \\
&\quad + \hat{c}_{6,\mathbf{k},\sigma}^{\dagger} \hat{c}_{4,\mathbf{k},\sigma} e^{+i\mathbf{k}(\mathbf{r}_6+\mathbf{a}-\mathbf{r}_4)}) + H.c.]. \tag{B1}
\end{aligned}$$

Introducing the notation $k\mathbf{a} = \mathbf{k}\mathbf{a} \in (-\pi, +\pi]$, $b = a/3$, where $a = |\mathbf{a}|$ is the lattice constant, and taking into account that

$$\begin{aligned}
\mathbf{k}\mathbf{r}_1 &= 0, \quad \mathbf{k}\mathbf{r}_2 = \frac{kb}{2}, \quad \mathbf{k}\mathbf{r}_3 = \frac{3kb}{2}, \quad \mathbf{k}\mathbf{r}_4 = 2kb, \\
\mathbf{k}\mathbf{r}_5 &= \frac{3kb}{2}, \quad \mathbf{k}\mathbf{r}_6 = \frac{kb}{2}, \quad \mathbf{k}\mathbf{r}_7 = 2kb, \quad \mathbf{k}\mathbf{r}_8 = \mathbf{k}\mathbf{a} = 3kb, \tag{B2}
\end{aligned}$$

\hat{H}_0 in \mathbf{k} space becomes of the form

$$\hat{H}_0 = \sum_{\sigma} \sum_{\mathbf{k}} \hat{\hat{C}}_{\mathbf{k},\sigma}^{\dagger} \tilde{M}_{\mathbf{k}} \hat{\hat{C}}_{\mathbf{k},\sigma}, \tag{B3}$$

where $\hat{\hat{C}}_{\mathbf{k},\sigma}^{\dagger}$ represents the eight component row vector $(\hat{c}_{1,\mathbf{k},\sigma}^{\dagger}, \hat{c}_{2,\mathbf{k},\sigma}^{\dagger}, \dots, \hat{c}_{8,\mathbf{k},\sigma}^{\dagger})$, $\hat{\hat{C}}_{\mathbf{k},\sigma}$ represents the eight component column vector obtained as the conjugate transpose of $\hat{\hat{C}}_{\mathbf{k},\sigma}^{\dagger}$, and $\tilde{M}_{\mathbf{k}}$ is a 8×8 Hermitian matrix whose transpose $\tilde{M}_{\mathbf{k}}^t$ is given by

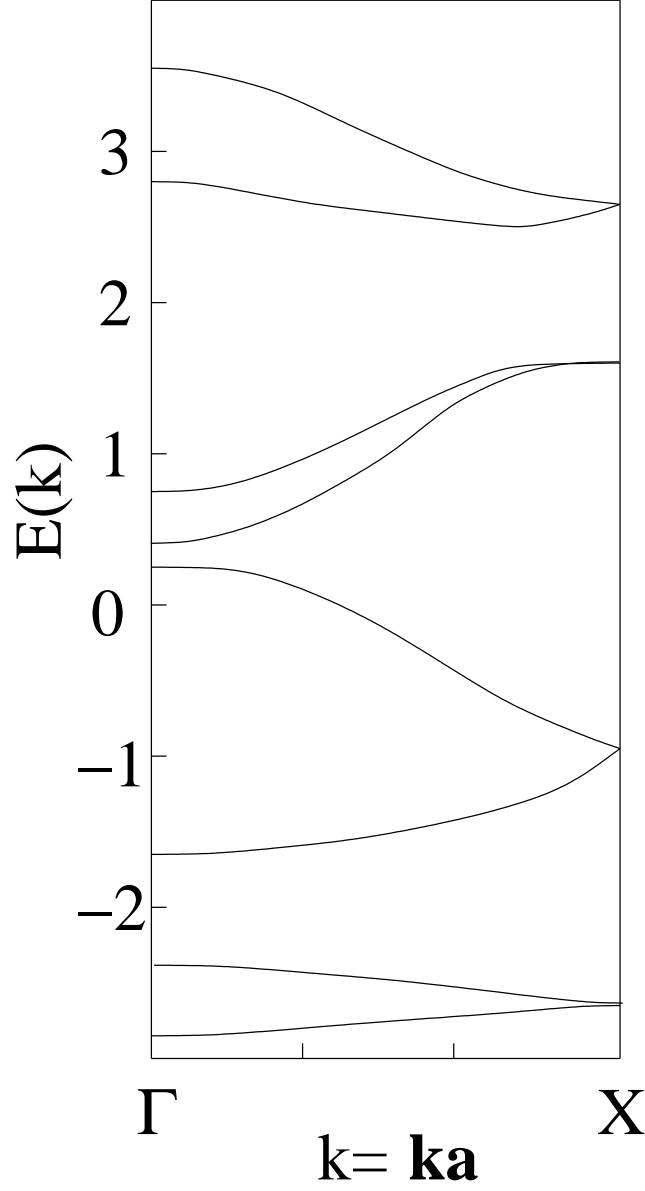


FIG. 11: Exemplification of the bare band structure at $t_2/t_1 = 1.2$, $t_3/t_1 = 1.3$, $t_4/t_1 = 1.05$, $t'_1/t_1 = 0.1$, $t'_2/t_1 = 0.2$, $\epsilon_0/t_1 = -0.9$, $\epsilon_1/t_1 = 1.15$, and $t_1 > 0$. The energy values are in t_1 units. Since $E(k = \mathbf{k}\mathbf{a})$ is even in k , only the $k \in [0, \pi]$ is shown. The folding at $k = \pi$ is a consequence of the structure of the cell.

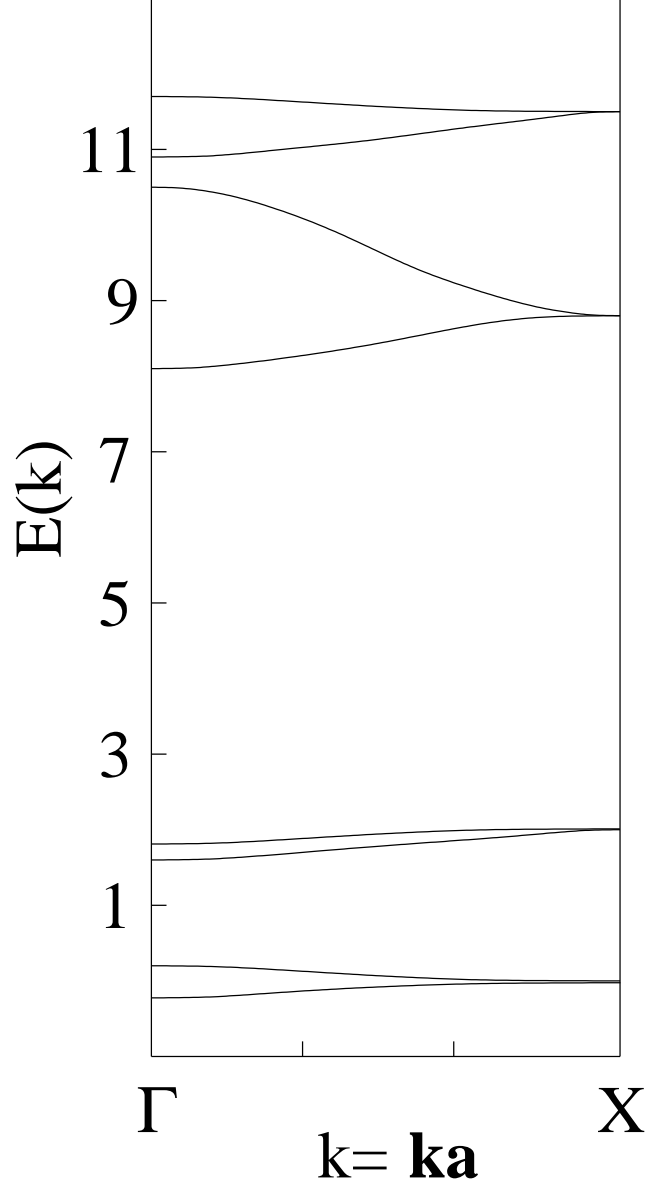


FIG. 12: The bare band structure in the presence of the condition (A11). One has $t_3/t_1 = 1.3$, $t_4/t_1 = 1.05$, $t'_1/t_1 = 0.1$, $t'_2/t_1 = 0.2$, $\epsilon_1/t_1 = 1.15$, $t_1 > 0$, and t_2, ϵ_0 are given by (A11). The energy values are in t_1 units. Since $E(k = \mathbf{k}\mathbf{a})$ is even in k , only the $k \in [0, \pi]$ is shown. The folding at $k = \pi$ is a consequence of the structure of the cell.

$$\tilde{M}_{\mathbf{k}}^t = \begin{pmatrix} \epsilon_0 & t_3 e^{ikb/2} & 2t'_1 \cos \frac{ak}{2} & t_2 e^{-ikb} & 2t'_2 \cos \frac{ak}{2} & t_1 e^{ikb/2} & 0 & t'_1 \\ t_3 e^{-ikb/2} & \epsilon_1 & t_4 e^{ikb} & 2t'_1 \cos \frac{ak}{2} & 0 & t'_1 & 0 & 0 \\ 2t'_1 \cos \frac{ak}{2} & t_4 e^{-ikb} & \epsilon_1 & t_3 e^{ikb/2} & t'_1 & 0 & 0 & 0 \\ t_2 e^{ikb} & 2t'_1 \cos \frac{ak}{2} & t_3 e^{-ikb/2} & \epsilon_0 & t_1 e^{-ikb/2} & 2t'_2 \cos \frac{ak}{2} & t'_1 & 0 \\ 2t'_2 \cos \frac{ak}{2} & 0 & t'_1 & t_1 e^{ikb/2} & \epsilon_0 & t_2 e^{-ikb} & t_3 e^{ikb/2} & 2t'_1 \cos \frac{ak}{2} \\ t_1 e^{-ikb/2} & t'_1 & 0 & 2t'_2 \cos \frac{ak}{2} & t_2 e^{ikb} & \epsilon_0 & 2t'_1 \cos \frac{ak}{2} & t_3 e^{-ikb/2} \\ 0 & 0 & 0 & t'_1 & t_3 e^{-ikb/2} & 2t'_1 \cos \frac{ak}{2} & \epsilon_1 & t_4 e^{ikb} \\ t'_1 & 0 & 0 & 0 & 2t'_1 \cos \frac{ak}{2} & t_3 e^{ikb/2} & t_4 e^{-ikb} & \epsilon_1 \end{pmatrix} \quad (\text{B4})$$

The bare band structure is obtained from the secular equation of $\tilde{M}_{\mathbf{k}}$ as an eight order algebraic equation in $\lambda = E_n(k)$, $n = 1, 2, \dots, 8$ of the form

$$\frac{1}{(e_1^2 - t_4^2)^2} \{ (E^2 - Z^2 - |W|^2 - |F|^2)^2 - Y^2 + 4Z[EY - Z(|W|^2 + |F|^2)] \} = 0, \quad (\text{B5})$$

where one has

$$\begin{aligned} |F|^2 &= |V|^2 + (|W|^2 + 2X) \cos^2 \frac{ak}{2}, \quad Y = 2(|W|^2 + X) \cos \frac{ak}{2}, \\ E &= e_0(e_1^2 - t_4^2) - e_1(t_1'^2 + t_3^2) - 4t'_1(t_1'e_1 - t_3t_4) \cos^2 \frac{ak}{2}, \\ Z &= 2[t_2'(e_1^2 - t_4^2) - 2t_1'^2 e_1 + t_3t_4t_1'] \cos \frac{ak}{2}, \quad X = \bar{d}(\bar{a} - \bar{b}) + 4t_4t_1'^2(\bar{a} - \bar{b} \cos^2 \frac{ak}{2}), \\ |W|^2 &= \bar{d}^2 + 8t_4t_1'^2 \bar{c} \cos^2 \frac{ak}{2}, \quad |V|^2 = \bar{a}^2 + \bar{b}(\bar{b} - 2\bar{a}) \cos^2 \frac{ak}{2}, \\ \bar{a} &= t_2(e_1^2 - t_4^2) + t_4(t_1'^2 - t_3^2), \quad \bar{b} = t_1(e_1^2 - t_4^2) + 2t_3(t_1'e_1 - t_3t_4), \\ \bar{c} &= t_1(e_1^2 - t_4^2) - 2t_1'(t_3e_1 - t_1't_4), \quad \bar{d} = t_1(e_1^2 - t_4^2) - 2t_3t_1'e_1, \\ e_0 &= \epsilon_0 - \lambda, \quad e_1 = \epsilon_1 - \lambda. \end{aligned} \quad (\text{B6})$$

An exemplification of the bare band structure is presented for the general case in Fig.11, while the bare band structure in the presence of the condition (A11) is exemplified in Fig.12. As Figs.(11,12) show, flat bands in the bare band structure are not present for non-zero values of all \hat{H}_0 parameters. This fact can be directly and analytically verified in the following way. The relation (B5) can be written as

$$A_8 \cos^8 \frac{ak}{2} + A_6 \cos^6 \frac{ak}{2} + A_4 \cos^4 \frac{ak}{2} + A_2 \cos^2 \frac{ak}{2} + A_0 = 0, \quad (\text{B7})$$

where the numerical prefactors A_{2m} , $m = 0, 1, \dots, 4$ are dependent only on \hat{H}_0 parameters and the eigenvalue λ . Since now in (B7) the entire k dependence is concentrated in the

$\cos^{2m}(ka/2)$ terms, it results that flat band solutions (i.e. k -independent expressions for λ) can be obtained only if for a given solution, simultaneously for all A_{2m} , $A_{2m} = 0$ holds. But, since one has $A_8 = (16t_1'^4)^2$, this condition cannot be satisfied for non-zero value of the hopping matrix elements. Consequently, the band structure created by \hat{H}_0 does not contain flat bands at all. One further notes that the $A_{2m < 8}$ prefactors can be as well easily calculated based on (B5,B6), and one finds that the denominator in (B5) simplifies in all A_{2m} . One obtains for example $A_0 = \{(e_1^2 - t_4^2)(e_0^2 - t_1^2 - t_2^2) + (t_1'^2 - t_3^2)^2 + 2[2t_1t_3t_1'e_1 - e_0e_1(t_1'^2 + t_3^2) - t_2t_4(t_1'^2 - t_3^2)]\}^2$, or $A_6 = -256t_1'^2\{t_1'^2t_2'^2e_1^2/2 - [t_2't_4(2t_2't_3 - t_1't_1) + t_1'^2(2t_1t_2' + t_2t_3)]e_1t_1' - t_1'^3t_3t_4e_0 + t_1'^4e_0e_1 + t_1'^4(t_1'^2 + t_3^2) + t_2't_3t_4^2(t_2't_3 - t_1't_1) + (t_1'^2t_4/4)[t_4(t_1^2 + 2t_2'^2) + 2t_3(4t_1't_2' + 2t_1t_2' + t_2t_3) - 4t_1'^2(t_1 - t_2)]\}$, etc.

Appendix C: Example for \hat{B}^\dagger operators

In this section one exemplifies solutions of (17) in the $m = 6$ case (i.e. the number of cells in the test chain is six) inside the parameter space region specified by

$$t_1' > 0, \quad t_3 = 3t_1', \quad 6t_1'^2 = t_4(t_1 - 4t_2'). \quad (\text{C1})$$

One further introduces the parameter $A = (t_1 - 4t_2')/(t_1 + 2t_2')$.

In this region one has a \hat{B}^\dagger solution holding the same coefficients in each cell, the solution being present at arbitrary $N_c = m$ and arbitrary A . This operator will be denoted by the $\ell = 1$ index, and has the expression

$$\hat{B}_{1,\sigma}^\dagger = \sum_{n=0}^{N_c-1} (\hat{c}_{\mathbf{j}+n\mathbf{a}+\mathbf{r}_5,\sigma}^\dagger - \hat{c}_{\mathbf{j}+n\mathbf{a}+\mathbf{r}_4,\sigma}^\dagger + \hat{c}_{\mathbf{j}+(n+1)\mathbf{a}+\mathbf{r}_1,\sigma}^\dagger - \hat{c}_{\mathbf{j}+(n+1)\mathbf{a}+\mathbf{r}_6,\sigma}^\dagger). \quad (\text{C2})$$

Given by its cell homogeneous nature, the \hat{B}^\dagger from (C2) cannot be translated or rotated in providing new, linearly independent \hat{B}^\dagger operators.

The following linearly independent solutions emerge for different A values from which

one presents below the $A = \sqrt{3}$ case. For this parameter region, $\hat{B}_{2,\sigma}^\dagger$ has the coefficients

$$\begin{aligned}
x_{2,1,1} &= \frac{1+\sqrt{3}}{2}, x_{2,1,2} = -\frac{1+\sqrt{3}}{2g}, x_{2,1,3} = -\frac{1+\sqrt{3}}{g}, x_{2,1,4} = 1, x_{2,1,5} = -1, \\
x_{2,1,6} &= -\frac{1+\sqrt{3}}{2}, x_{2,1,7} = \frac{3+\sqrt{3}}{2g}, x_{2,1,8} = \frac{3+\sqrt{3}}{2g}, \\
x_{2,2,1} &= \sqrt{3}, x_{2,2,2} = -\frac{1+\sqrt{3}}{g}, x_{2,2,3} = -\frac{1+\sqrt{3}}{2g}, x_{2,2,4} = \frac{3-\sqrt{3}}{2}, x_{2,2,5} = -\frac{3-\sqrt{3}}{2}, \\
x_{2,2,6} &= -\sqrt{3}, x_{2,2,7} = \frac{3+\sqrt{3}}{2g}, x_{2,2,8} = 0, \\
x_{2,3,1} &= -(1-\sqrt{3}), x_{2,3,2} = -\frac{1+\sqrt{3}}{2g}, x_{2,3,3} = \frac{1+\sqrt{3}}{2g}, x_{2,3,4} = 1-\sqrt{3}, x_{2,3,5} = -(1-\sqrt{3}), \\
x_{2,3,6} &= 1-\sqrt{3}, x_{2,3,7} = 0, x_{2,3,8} = -\frac{3+\sqrt{3}}{2g}, \\
x_{2,4,1} &= -\frac{3-\sqrt{3}}{2}, x_{2,4,2} = \frac{1+\sqrt{3}}{2g}, x_{2,4,3} = \frac{1+\sqrt{3}}{g}, x_{2,4,4} = -\sqrt{3}, x_{2,4,5} = \sqrt{3}, \\
x_{2,4,6} &= \frac{3-\sqrt{3}}{2}, x_{2,4,7} = -\frac{3+\sqrt{3}}{2g}, x_{2,4,8} = -\frac{3+\sqrt{3}}{2g}, \\
x_{2,5,1} &= -1, x_{2,5,2} = \frac{1+\sqrt{3}}{g}, x_{2,5,3} = \frac{1+\sqrt{3}}{2g}, x_{2,5,4} = -\frac{1+\sqrt{3}}{2}, x_{2,5,5} = \frac{1+\sqrt{3}}{2}, \\
x_{2,5,6} &= 1, x_{2,5,7} = -\frac{3+\sqrt{3}}{2g}, x_{2,5,8} = 0, \\
x_{2,6,1} &= 0, x_{2,6,2} = \frac{1+\sqrt{3}}{2g}, x_{2,6,3} = -\frac{1+\sqrt{3}}{2g}, x_{2,6,4} = 0, x_{2,6,5} = 0, \\
x_{2,6,6} &= 0, x_{2,6,7} = 0, x_{2,6,8} = \frac{3+\sqrt{3}}{2g},
\end{aligned} \tag{C3}$$

where $g = 6t'_1/(t_1 + 2t'_2)$ is arbitrary. This solution can be translated five times by \mathbf{a} obtaining $\hat{B}_{3,\sigma}^\dagger, \hat{B}_{4,\sigma}^\dagger, \dots, \hat{B}_{7,\sigma}^\dagger$, and the six operators $\hat{B}_{2,\sigma}^\dagger, \dots, \hat{B}_{7,\sigma}^\dagger$ can be rotated by π obtaining $\hat{B}_{8,\sigma}^\dagger, \dots, \hat{B}_{13,\sigma}^\dagger$. Consequently, at this moment, the number of linearly independent \hat{B}^\dagger operators with fixed spin at our disposal is 13.

The following linearly independent solution holding the index $\ell = 14$ has the prefactors

$$\begin{aligned}
x_{14,1,1} &= \sqrt{3}, x_{14,1,2} = -\frac{\sqrt{3}}{g}, x_{14,1,3} = -\frac{\sqrt{3}}{g}, x_{14,1,4} = 2 - \sqrt{3}, x_{14,1,5} = -(2 - \sqrt{3}), \\
x_{14,1,6} &= -\sqrt{3}, x_{14,1,7} = \frac{2}{g}, x_{14,1,8} = \frac{1}{g}, \\
x_{14,2,1} &= -2(1 - \sqrt{3}), x_{14,2,2} = -\frac{\sqrt{3}}{g}, x_{14,2,3} = 0, x_{14,2,4} = 3 - 2\sqrt{3}, x_{14,2,5} = -(3 - 2\sqrt{3}), \\
x_{14,2,6} &= 2(1 - \sqrt{3}), x_{14,2,7} = \frac{1}{g}, x_{14,2,8} = -\frac{1}{g}, \\
x_{14,3,1} &= -(3 - 2\sqrt{3}), x_{14,3,2} = 0, x_{14,3,3} = \frac{\sqrt{3}}{g}, x_{14,3,4} = 2(1 - \sqrt{3}), x_{14,3,5} = -2(1 - \sqrt{3}), \\
x_{14,3,6} &= 3 - 2\sqrt{3}, x_{14,3,7} = -\frac{1}{g}, x_{14,3,8} = -\frac{2}{g}, \\
x_{14,4,1} &= -(2 - \sqrt{3}), x_{14,4,2} = \frac{\sqrt{3}}{g}, x_{14,4,3} = \frac{\sqrt{3}}{g}, x_{14,4,4} = -\sqrt{3}, x_{14,4,5} = \sqrt{3}, \\
x_{14,4,6} &= 2 - \sqrt{3}, x_{14,4,7} = -\frac{2}{g}, x_{14,4,8} = -\frac{1}{g}, \\
x_{14,5,1} &= 0, x_{14,5,2} = \frac{\sqrt{3}}{g}, x_{14,5,3} = 0, x_{14,5,4} = -1, x_{14,5,5} = 1, \\
x_{14,5,6} &= 0, x_{14,5,7} = -\frac{1}{g}, x_{14,5,8} = \frac{1}{g}, \\
x_{14,6,1} &= 1, x_{14,6,2} = 0, x_{14,6,3} = -\frac{\sqrt{3}}{g}, x_{14,6,4} = 0, x_{14,6,5} = 0, \\
x_{14,6,6} &= -1, x_{14,6,7} = \frac{1}{g}, x_{14,6,8} = \frac{2}{g}.
\end{aligned} \tag{C4}$$

Similarly, another linearly independent $\hat{B}_{\ell,\sigma}^\dagger$ term $\ell = 15$ is the following one

$$\begin{aligned}
x_{15,1,1} &= \frac{3 - \sqrt{3}}{2}, x_{15,1,2} = -\frac{1 - \sqrt{3}}{2g}, x_{15,1,3} = -\frac{1}{g}, x_{15,1,4} = -(2 - \sqrt{3}), x_{15,1,5} = 2 - \sqrt{3}, \\
x_{15,1,6} &= -\frac{3 - \sqrt{3}}{2}, x_{15,1,7} = -\frac{1 - \sqrt{3}}{2g}, x_{15,1,8} = \frac{1 + \sqrt{3}}{2g}, \\
x_{15,2,1} &= 3 - \sqrt{3}, x_{15,2,2} = -\frac{1}{g}, x_{15,2,3} = -\frac{1 + \sqrt{3}}{2g}, x_{15,2,4} = -\frac{5 - 3\sqrt{3}}{2}, x_{15,2,5} = \frac{5 - 3\sqrt{3}}{2}, \\
x_{15,2,6} &= -(3 - \sqrt{3}), x_{15,2,7} = \frac{1 + \sqrt{3}}{2g}, x_{15,2,8} = \frac{1}{g}, \\
x_{15,3,1} &= 3 - \sqrt{3}, x_{15,3,2} = -\frac{1 + \sqrt{3}}{2g}, x_{15,3,3} = \frac{1 - \sqrt{3}}{2g}, x_{15,3,4} = -(2 - \sqrt{3}), x_{15,3,5} = 2 - \sqrt{3}, \\
x_{15,3,6} &= -(3 - \sqrt{3}), x_{15,3,7} = \frac{1}{g}, x_{15,3,8} = \frac{1 - \sqrt{3}}{2g}, \\
x_{15,4,1} &= \frac{3 - \sqrt{3}}{2}, x_{15,4,2} = \frac{1 - \sqrt{3}}{2g}, x_{15,4,3} = \frac{1}{g}, x_{15,4,4} = -1, x_{15,4,5} = 1, \\
x_{15,4,6} &= -\frac{3 - \sqrt{3}}{2}, x_{15,4,7} = \frac{1 - \sqrt{3}}{2g}, x_{15,4,8} = -\frac{1 + \sqrt{3}}{2g}, \\
x_{15,5,1} &= 0, x_{15,5,2} = \frac{1}{g}, x_{15,5,3} = \frac{1 + \sqrt{3}}{2g}, x_{15,5,4} = -\frac{1 + \sqrt{3}}{2}, x_{15,5,5} = \frac{1 + \sqrt{3}}{2}, \\
x_{15,5,6} &= 0, x_{15,5,7} = -\frac{1 + \sqrt{3}}{2g}, x_{15,5,8} = -\frac{1}{g}, \\
x_{15,6,1} &= 0, x_{15,6,2} = \frac{1 + \sqrt{3}}{2g}, x_{15,6,3} = -\frac{1 - \sqrt{3}}{2g}, x_{15,6,4} = -1, x_{15,6,5} = 1, \\
x_{15,6,6} &= 0, x_{15,6,7} = -\frac{1}{g}, x_{15,6,8} = -\frac{1 - \sqrt{3}}{2g}. \tag{C5}
\end{aligned}$$

Both $\hat{B}_{14,\sigma}^\dagger$, and $\hat{B}_{15,\sigma}^\dagger$ can be translated and rotated in providing new \hat{B}^\dagger operators in the ground state wave vector, but from these not all are linearly independent.

One further note that maintaining (C1), solutions can be found also for other A values, as for example $A = 0.75, 1, 2, 4, \sqrt{2}, (\sqrt{5} \pm 1)/2$, etc. Furthermore, solutions are present even if (C1) does not hold, but in this case cell homogeneous \hat{B}^\dagger operators as presented in (C2), are not present.

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